

Supporting information

Salt-Induced Thermochromism of a Conjugated Polyelectrolyte

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1. Stationary absorption spectra of CPT in PBS at different concentrations

Figure S1 shows the normalized absorption spectra of CPT in PBS buffer solution at different concentrations at four temperatures (5, 25, 40 and 55°C). The shape is almost completely independent from the concentration in the investigated range.

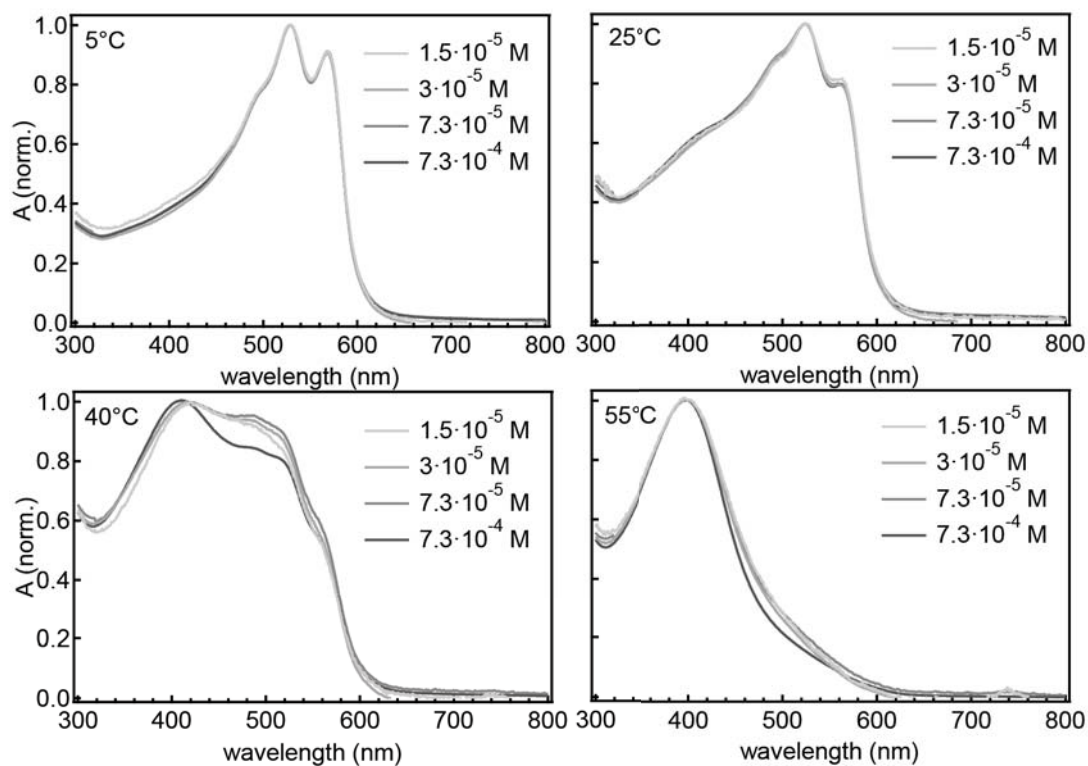


Figure S1 Normalized absorption spectra of CPT in PBS at different monomeric concentrations (from $1.5 \cdot 10^{-5}$ M to $7.3 \cdot 10^{-4}$ M) at four different temperatures (5, 25, 40 and 55°C)

2. Solvatochromism of CPT in various solvents

Figure S2 shows the stationary absorption spectra of CPT at room temperature in various solvents and solvent mixtures. The absorption is red shifted for solvents with higher refractive index, pointing to a predominant effect due to dispersion interactions.

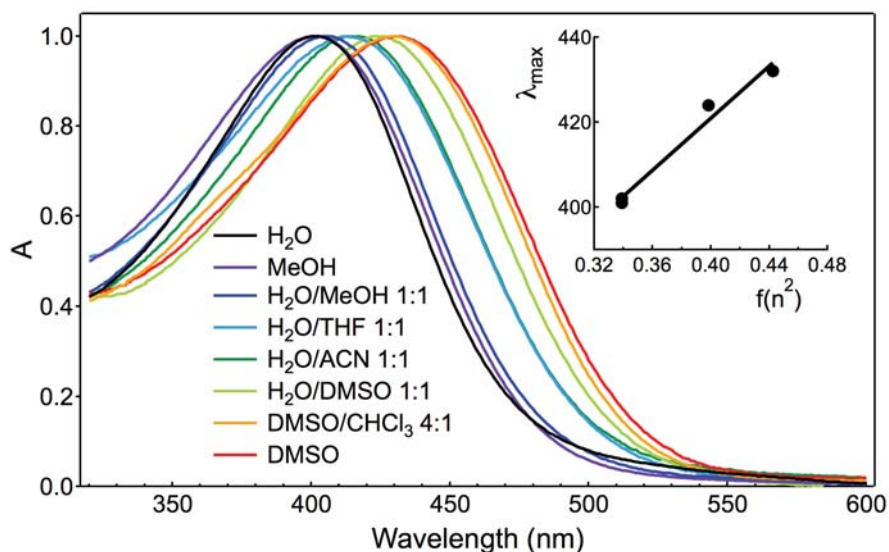


Figure S2 Normalized absorption spectra of CPT in various solvents and solvent mixtures at room temperature. The inset shows the absorption maximum as a function of the solvent Onsager refractive index function $f(n^2) = 2(n^2-1)/(2n^2+1)$, for H₂O ($n=1.33$), MeOH ($n=1.33$), H₂O/DMSO ($n=1.41$) and DMSO ($n=1.48$).

3. Stationary absorption spectra of CPT in different aqueous salt solutions

Figure S3 shows the absorption spectra of CPT at room temperature in pure water, in PBS and in different salt solutions. The main effect on the red-shifted absorption of CPT in PBS is due to the Cl^- anions present in the buffer.

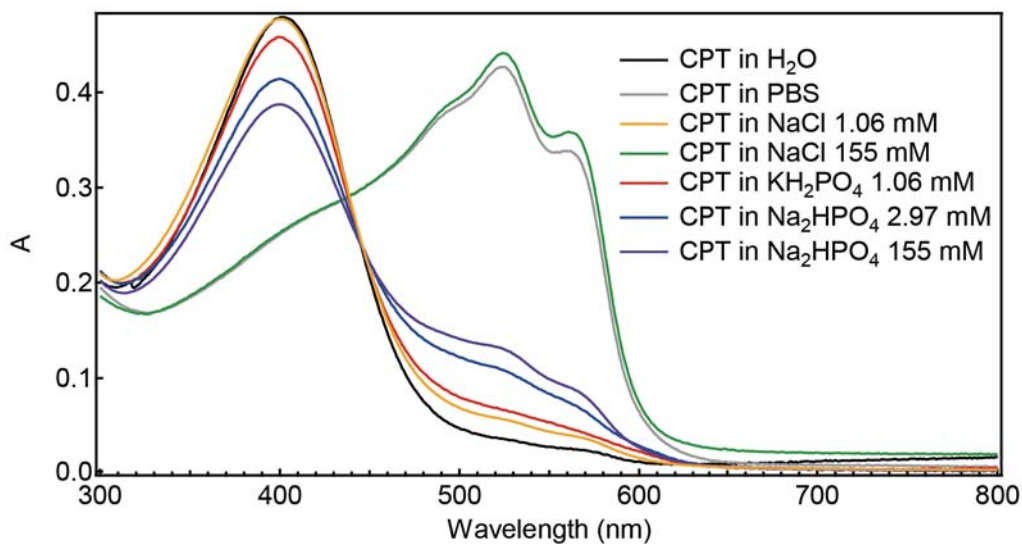


Figure S3 Absorption spectra of CPT ($7.3 \cdot 10^{-5}$ M, monomeric basis) at 25°C in water, in PBS and in different aqueous salt solutions.

4. Stationary absorption spectra of CPT in PBS for different temperature ranges

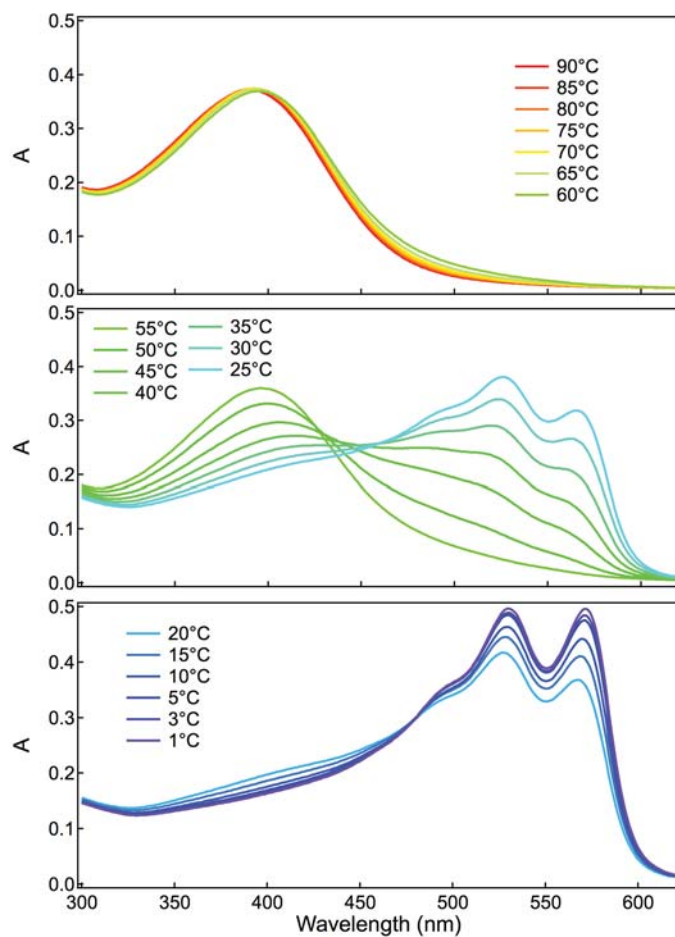


Figure S4 Absorption spectra of CPT ($7.3 \cdot 10^{-5}$ M, monomeric basis) in PBS at different temperatures between 1°C and 90°C, shown for clarity for different temperature ranges.

5. Stationary absorption spectra of CPT in PBS: increasing and decreasing temperature

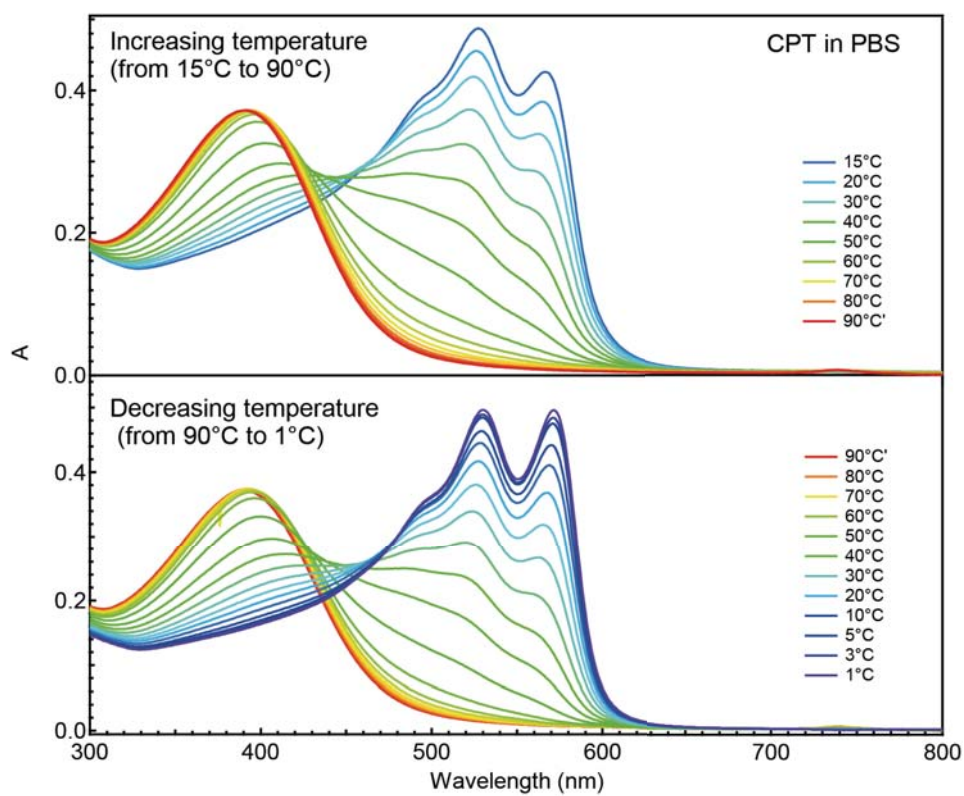


Figure S5 Absorption spectra of CPT in PBS ($7.3 \cdot 10^{-5}$ M, monomeric basis). Top: upon heating from 15 to 90°C. Bottom: upon cooling from 90 to 1°C.

6. Stationary absorption spectra of CPT in pure water, with decreasing temperature

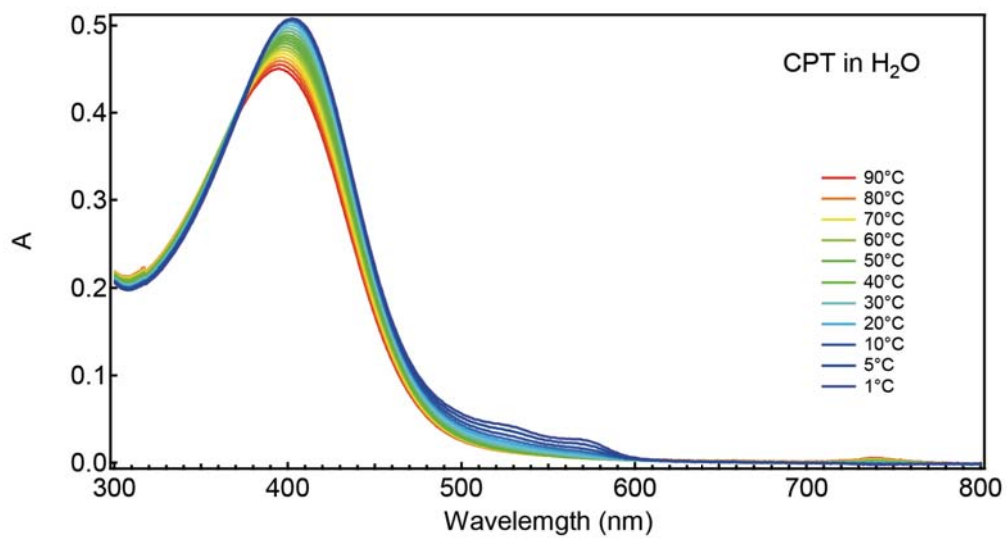


Figure S6 Absorption spectra of CPT in pure water ($7.3 \cdot 10^{-5}$ M, monomeric basis) upon decreasing temperature from 90 to 1°C.

7. Resonance Raman spectra

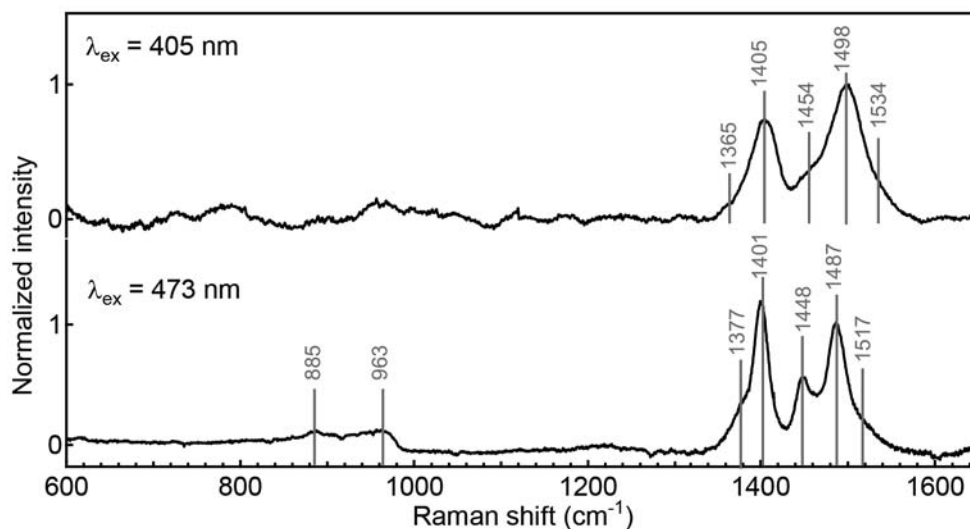


Figure S7 Experimental Resonance Raman spectra of CPT in PBS solution ($1.5 \cdot 10^{-4}$ M, monomeric basis) at room temperature excited at 405 nm and 473 nm. They are shown over an extended range compared to the main text.

8. Computed Raman spectra and coordinates for the optimized and scan structures

8.1 Computed Raman Spectra

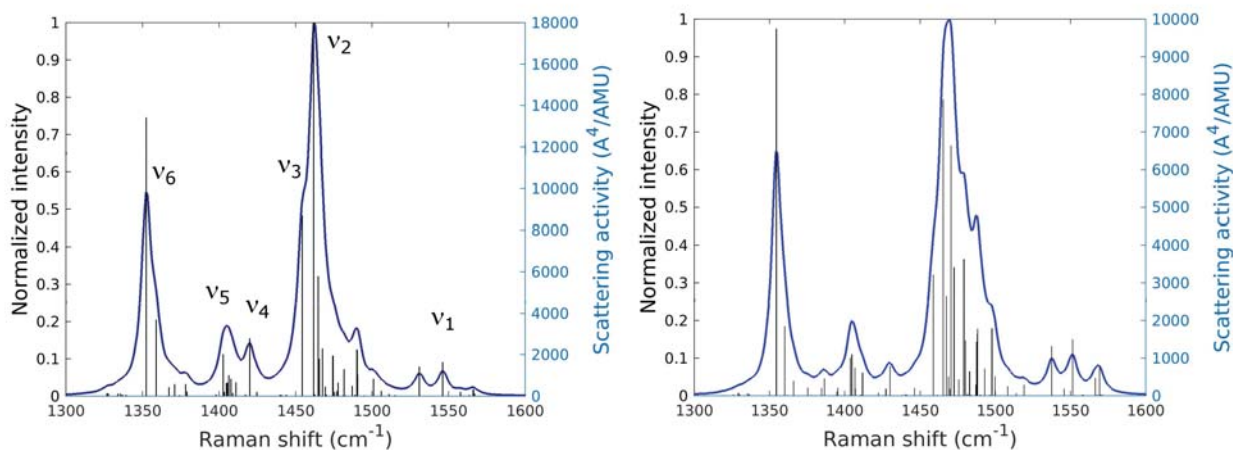


Figure S8.1: Raman spectra featuring both individual and convoluted (4 cm^{-1}) vibrational modes of CPT scan at $\theta=0^\circ$ (left) and $\theta=20^\circ$ (right), computed at the B3LYP-D3(BJ)/6-31G* level, applying the 0.97 scaling factor for B3LYP.

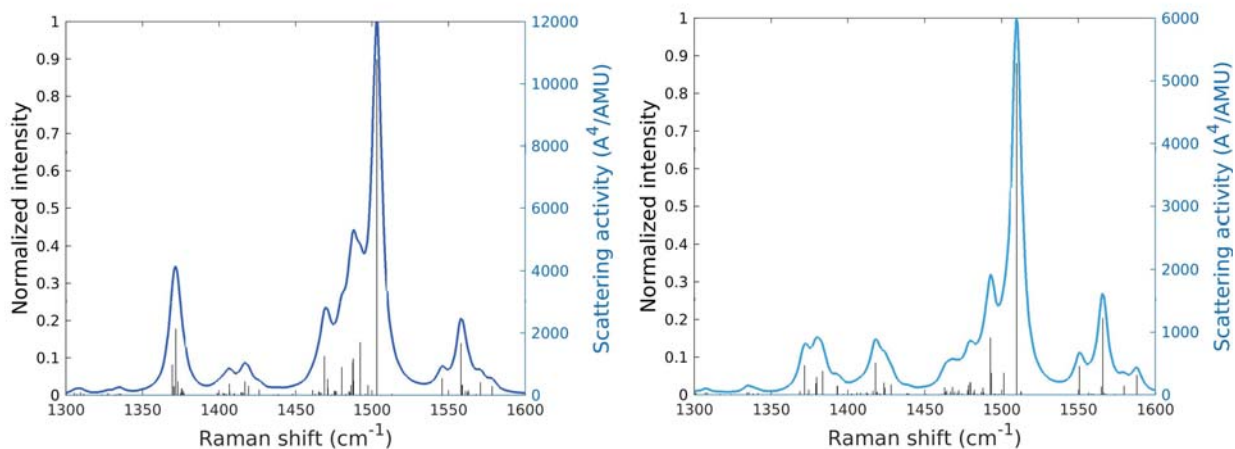


Figure S8.2: Raman spectra featuring both individual and convoluted (4 cm^{-1}) vibrational modes of CPT scan at $\theta=40^\circ$ (left) and $\theta=60^\circ$ (right), computed at the B3LYP-D3(BJ)/6-31G* level, applying the 0.97 scaling factor for B3LYP.

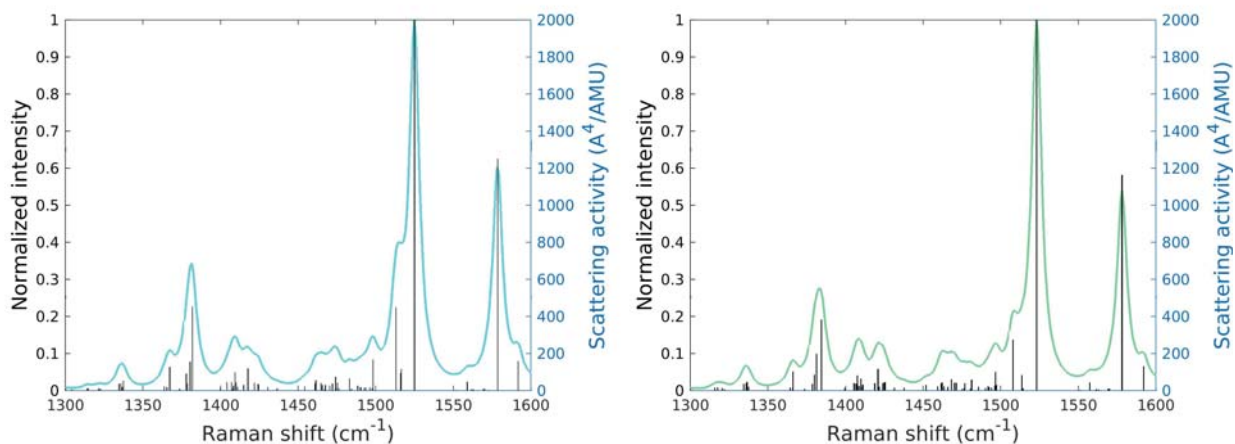


Figure S8.3: Raman spectra featuring both individual and convoluted (4 cm^{-1}) vibrational modes of CPT scan at $\theta=80^\circ$ (left) and $\theta=90^\circ$ (right), computed at the B3LYP-D3(BJ)/6-31G* level, applying the 0.97 scaling factor for B3LYP.

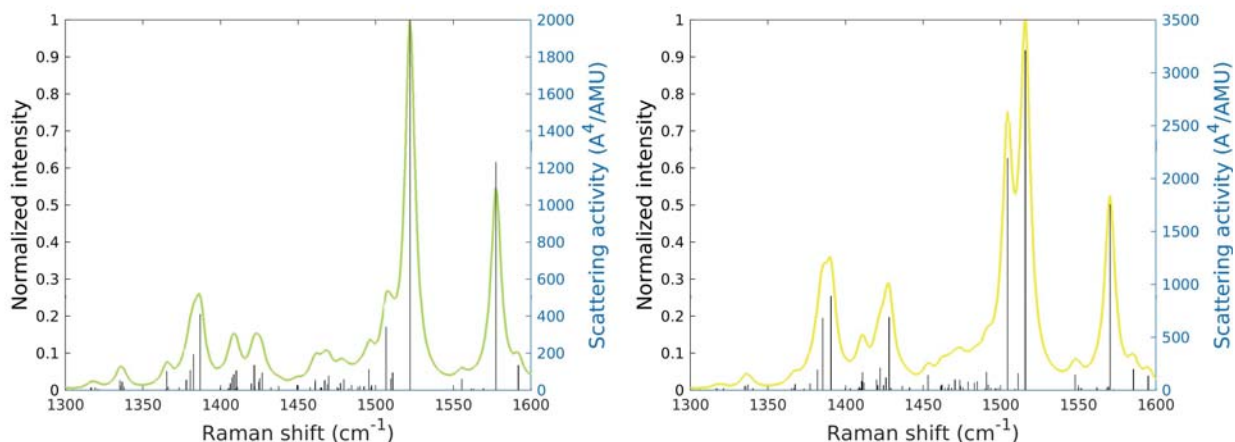


Figure S8.4: Raman spectra featuring both individual and convoluted (4 cm^{-1}) vibrational modes of CPT scan at $\theta=100^\circ$ (left) and $\theta=120^\circ$ (right), computed at the B3LYP-D3(BJ)/6-31G* level, applying the 0.97 scaling factor for B3LYP.

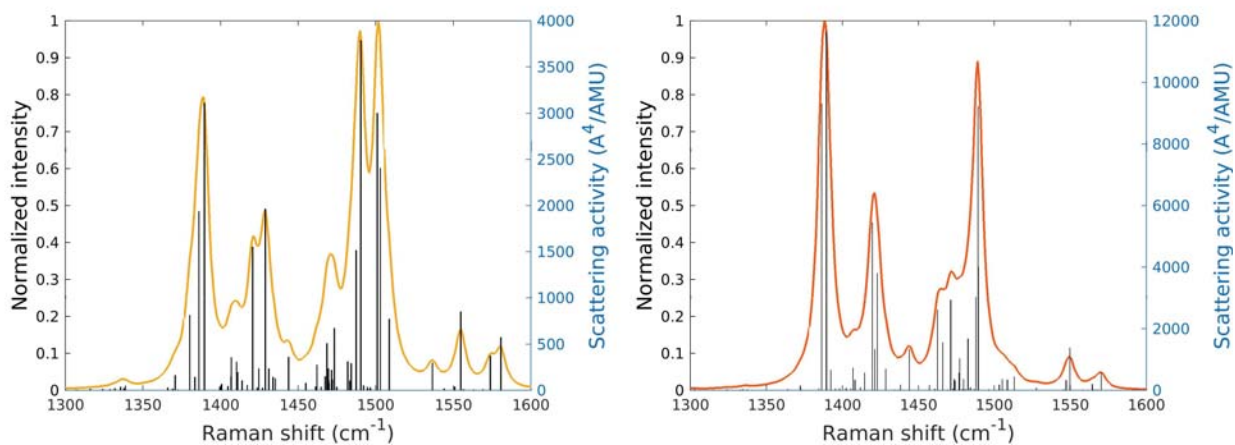


Figure S8.5: Raman spectra featuring both individual and convoluted (4 cm^{-1}) vibrational modes of CPT scan at $\theta=140^\circ$ (left) and $\theta=160^\circ$ (right), computed at the B3LYP-D3(BJ)/6-31G* level, applying the 0.97 scaling factor for B3LYP.

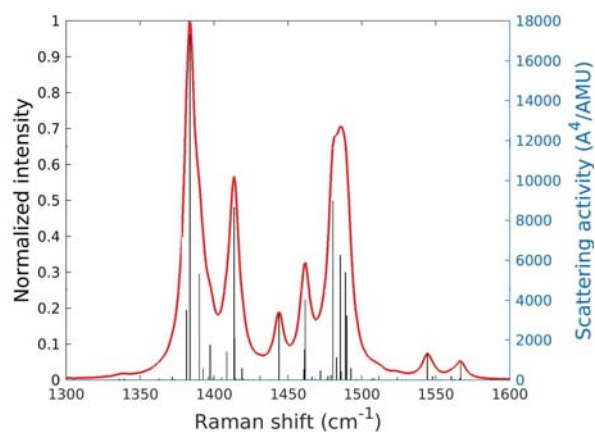


Figure S8.6: Raman spectrum featuring both individual and convoluted (4 cm^{-1}) vibrational modes of CPT scan at $\theta=180^\circ$, computed at the B3LYP-D3(BJ)/6-31G* level, applying the 0.97 scaling factor for B3LYP.

8.2 Optimized structures

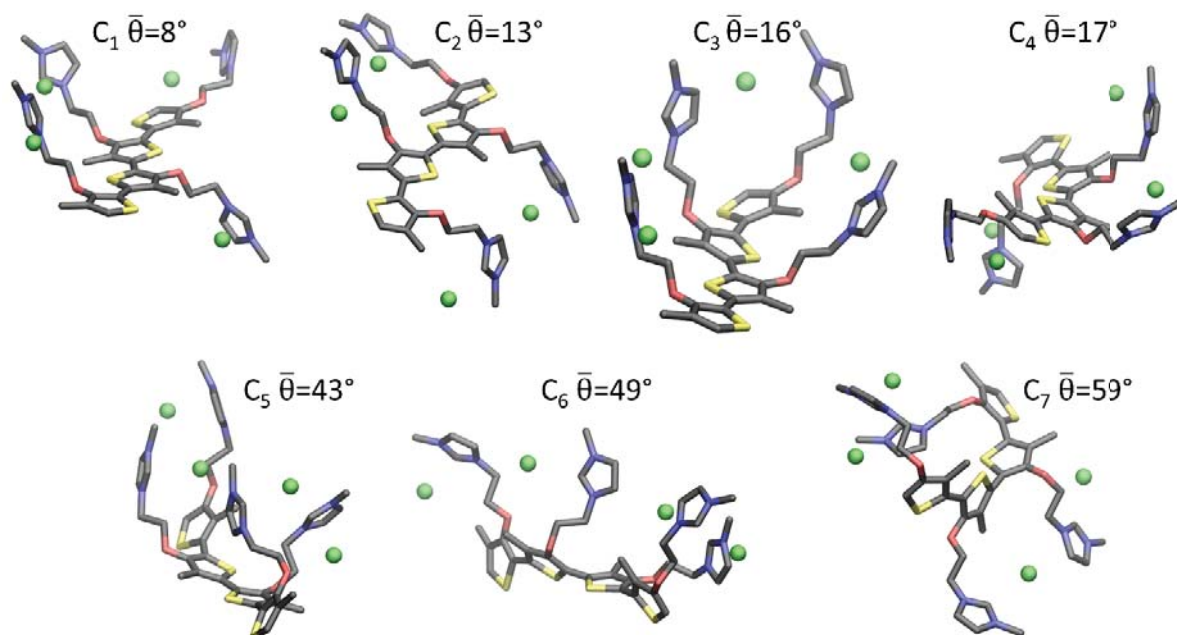


Figure S8.7: 3D representations of geometries optimized at the B3LYP-D3(BJ)/6-31G*. Starting geometries were randomly generated with seven distinct θ dihedral angles. Only the mean dihedral angle, mapped in the $[0,90]$ range, is shown.

8.3 Coordinates of dihedral scan

Geometries optimized at the B3LYP-D3(BJ)/6-31G(d) level with all three $\theta = \angle \text{SCCS}$ angles frozen at the angle corresponding to output name (20.log means $\theta = 20^\circ$)

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118
0.log Energy: -3690946.1754128 Ha
C      -6.62434      -4.03393      -0.60993
C      -5.85475      -2.84884      -0.87374
C      -5.81208      -5.09500      -0.33044
C      -4.47748      -3.01951      -0.84969
S      -4.12988      -4.69263      -0.40317
H      -6.11017      -6.10894      -0.10072
C      -8.12473      -4.07866      -0.64489
H      -8.56524      -3.80644       0.32525
H      -8.47344      -5.08700      -0.88788
H      -8.50926      -3.39218      -1.40768
O      -6.47801      -1.65901      -1.15097
C      -7.08687      -1.01516      -0.02598
C      -8.22872      -0.17191      -0.59023
H      -6.35188      -0.37445       0.47807
H      -7.45821      -1.75618       0.69119
N      -9.03313       0.39014       0.50300
H      -8.87387      -0.79954      -1.20981
H      -7.84477       0.66334      -1.17991
C      -9.71515      -0.35825       1.38153
N     -10.27945       0.46488       2.27134
C      -9.95629       1.77551       1.94484
C      -9.16769       1.73146       0.83329
H      -8.65856       2.49131       0.25017
H     -10.31134       2.60973       2.52842
H      -9.73224      -1.45847       1.48776
C     -11.06064      -0.00628       3.41639
H     -10.87290      -1.08118       3.52052
H     -12.12382       0.18672       3.24895
H     -10.72720       0.51972       4.31385
C      -3.26681      -0.79221      -1.46113
C      -1.90493      -0.33910      -1.48926
C      -3.36770      -2.08847      -0.97449
C      -0.93938      -1.27529      -1.15834
S      -1.76129      -2.74531      -0.65969
C      -4.35691       0.08601      -2.01243
H      -4.92584       0.61928      -1.24171
H      -5.07803      -0.49095      -2.58865
H      -3.91014       0.84131      -2.66503
O      -1.61294       0.95588      -1.84904
C      -1.91318       1.92425      -0.84120
C      -2.03304       3.26819      -1.55774
H      -1.11236       1.95567      -0.09306
H      -2.86021       1.67641      -0.34798
N      -2.70856       4.25100      -0.70054
H      -2.63485       3.14385      -2.46020
H      -1.04858       3.66445      -1.81056
C      -4.04050       4.36927      -0.60639
N      -4.30758       5.30530       0.31186
C      -3.11129       5.79372       0.81752
C      -2.10260       5.12910       0.18638
H      -1.02079       5.16662       0.26490
H      -3.08811       6.56399       1.57162
H      -4.81661       3.79436      -1.12503
C      -5.65689       5.72617       0.69488
H      -6.36829       5.05605       0.20131
H      -5.82113       6.75973       0.37910
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C	2.90086	-2.01595	-0.62336
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H	5.38433	-1.57072	-2.24527
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C	9.68414	-2.83104	0.20939
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H	7.88668	-1.69603	0.58790
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H	9.62806	-2.72919	-0.87594
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C	11.15442	-1.75433	1.98066
H	11.09728	-2.59408	2.65413
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C	11.79160	1.57169	0.68433
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Cl	1.08129	4.31700	-0.30023
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20.log Energy: -3690927.6898623 Ha

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H	-7.00135	-5.47743	1.23919
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H	-6.37716	-5.68641	-0.40696
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C	-6.68361	-2.64923	-0.10962
C	-7.57490	-2.33485	-1.31070
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N	-8.94581	-2.04298	-0.86878
H	-7.59521	-3.19666	-1.98337
H	-7.22007	-1.45563	-1.85382
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C	-9.64859	-0.86754	-1.09692
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H	-9.41898	-3.83917	0.32250
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C	-1.84035	0.04897	-0.69952
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C	-0.61218	-0.46002	-0.30961
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H	-4.27900	0.39927	-1.68865
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C	-3.06991	3.39351	-1.41500
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H	-3.55137	1.81119	-0.01931
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H	-6.09395	6.15939	0.81161
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C	2.76690	1.20874	-0.43847
C	0.76137	0.01251	-0.39515
C	3.31822	-0.05184	-0.30100

S	2.01558	-1.22343	-0.28292
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C	4.68990	-0.51635	-0.41295
C	6.67569	-2.02176	-0.78725
S	4.96724	-2.13507	-1.05289
H	7.32537	-2.84707	-1.04336
C	6.04460	1.35305	0.74009
H	6.02298	2.21119	0.05949
H	7.00237	1.36023	1.26707
H	5.24516	1.48683	1.47623
O	8.24575	-0.37658	0.11766
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C	10.54720	-0.72356	0.49278
H	9.44054	-1.38105	-1.25664
H	9.08620	-2.29360	0.21034
N	11.73617	-1.48196	0.10942
H	10.45001	-0.75181	1.58113
H	10.70272	0.31705	0.19600
C	12.08206	-2.68124	0.61276
N	13.15901	-3.12474	-0.05888
C	13.40652	-2.25659	-1.11345
C	12.52297	-1.23156	-1.01041
H	12.38921	-0.34395	-1.60711
H	14.19304	-2.44484	-1.82605
H	11.68293	-3.11654	1.51054
C	13.65962	-4.49107	0.06025
H	13.93692	-4.69393	1.09705
H	14.53907	-4.59741	-0.57591
H	12.85074	-5.16139	-0.25263
Cl	-9.32610	-4.91537	2.14599
Cl	-7.30756	1.23781	-2.22709
Cl	-0.99238	5.67333	0.42283
Cl	10.30121	-4.47382	-0.29519

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40.log Energy: -3690959.4860809 Ha

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C	-6.20670	-4.85101	0.25983

C	-4.68110	-2.88260	0.48458
S	-4.60473	-4.59575	0.87052
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C	-8.13596	-3.67018	-0.89182
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H	-8.41866	-4.66996	-1.23469
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C	-7.92397	0.13477	-1.21845
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H	-8.07226	-1.38179	0.32763
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H	-7.17984	0.84253	-1.58793
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H	-12.47859	1.53928	1.60049
H	-12.45890	-0.05430	0.78131
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C	-2.00679	-0.36197	1.22742
C	-3.50511	-2.04962	0.65726
C	-1.09827	-1.28015	0.73599
S	-1.94348	-2.71858	0.20052
C	-4.49469	0.03377	1.76800
H	-4.13028	0.63244	2.60941
H	-5.29688	-0.61730	2.12740
H	-4.92015	0.72091	1.02594
O	-1.59944	0.84032	1.75179
C	-1.93387	2.00295	0.99190
C	-1.18435	1.99774	-0.34418
H	-1.59798	2.85083	1.59144
H	-3.01597	2.07052	0.82730
N	-1.60788	3.14739	-1.15524
H	-1.39567	1.08412	-0.90459
H	-0.11293	2.09038	-0.16676
C	-2.81881	3.26831	-1.71581
N	-2.89640	4.47806	-2.28296
C	-1.69859	5.14639	-2.07602
C	-0.88964	4.31578	-1.35942
H	0.08819	4.43913	-0.90907
H	-1.53919	6.14715	-2.44380
H	-3.66013	2.58505	-1.62500
C	-4.08968	4.99802	-2.95203
H	-4.95525	4.46675	-2.54283
H	-4.01161	4.84790	-4.03236
H	-4.17293	6.06427	-2.73337
C	1.26447	-0.75726	1.57267
C	2.60763	-0.96903	1.12066
C	0.34414	-1.19641	0.64028
C	2.72824	-1.56150	-0.12056
S	1.13533	-1.84734	-0.79210
C	0.94364	-0.19594	2.92505
H	0.01973	-0.63069	3.31494
H	0.79314	0.88831	2.87930
H	1.76110	-0.40873	3.62110

O	3.70046	-0.67336	1.90403
C	4.07075	0.70130	1.94148
C	4.92410	1.04974	0.71478
H	4.66081	0.83532	2.85206
H	3.18373	1.34561	1.98966
N	5.28711	2.47383	0.76813
H	4.36597	0.86660	-0.20597
H	5.84944	0.47138	0.70303
C	4.39900	3.46713	0.63915
N	5.02474	4.62092	0.89768
C	6.35393	4.35384	1.19595
C	6.52016	3.00191	1.12306
H	7.37040	2.34618	1.27991
H	7.05012	5.14168	1.43530
H	3.31689	3.38403	0.48072
C	4.35570	5.92316	0.90559
H	4.63334	6.49343	0.01499
H	4.65578	6.47008	1.80184
H	3.27696	5.74101	0.92804
C	5.04956	-2.59146	-0.38343
C	5.96018	-2.87720	-1.45790
C	3.92678	-1.93406	-0.84490
C	5.54713	-2.45169	-2.69030
S	4.00156	-1.67379	-2.58781
H	6.04013	-2.60630	-3.63942
C	5.28129	-3.06138	1.02138
H	5.83060	-2.32023	1.61280
H	5.86138	-3.99000	1.01080
H	4.33193	-3.24107	1.53109
O	7.10335	-3.63002	-1.27661
C	8.19002	-2.94337	-0.66618
C	9.02398	-2.28451	-1.77440
H	8.78496	-3.69651	-0.14010
H	7.86348	-2.18369	0.05139
N	10.19258	-1.60138	-1.21493
H	8.41855	-1.54309	-2.30034
H	9.36481	-3.03076	-2.49640
C	10.24136	-0.29788	-0.91565
N	11.37276	-0.05532	-0.24118
C	12.03609	-1.25740	-0.04648
C	11.30083	-2.22545	-0.65600
H	11.46544	-3.28604	-0.75635
H	12.96642	-1.30926	0.49562
H	9.49953	0.43246	-1.18271
C	11.64987	1.20875	0.43928
H	11.65059	2.02642	-0.28460
H	12.63085	1.14300	0.91026
H	10.86214	1.35889	1.18496
Cl	-11.22222	-2.37102	0.66254
Cl	-5.77591	2.81579	-0.77795
Cl	1.33326	3.89334	1.09699
Cl	8.39449	0.18358	1.18001

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60.log Energy: -3690958.6247551 Ha

C	-7.49216	-3.01510	-1.21135
C	-6.38402	-2.16281	-0.85668
C	-7.29796	-4.28493	-0.74265
C	-5.36783	-2.79880	-0.17598
S	-5.79515	-4.47985	0.10124
H	-7.95900	-5.13209	-0.86820
C	-8.66007	-2.57645	-2.04840
H	-9.45953	-2.09090	-1.47180

H	-9.10908	-3.43449	-2.55763
H	-8.32967	-1.86541	-2.81490
O	-6.29521	-0.85244	-1.24896
C	-7.26654	0.02220	-0.66235
C	-7.42928	1.19887	-1.61786
H	-6.90729	0.38398	0.30536
H	-8.22401	-0.48935	-0.52157
N	-8.46469	2.10420	-1.10457
H	-7.73581	0.84677	-2.60556
H	-6.49523	1.75853	-1.68466
C	-9.77529	1.82068	-1.12857
N	-10.41705	2.78976	-0.46626
C	-9.48984	3.71689	-0.00996
C	-8.25848	3.28432	-0.40288
H	-7.25329	3.64949	-0.22792
H	-9.78750	4.58630	0.55392
H	-10.27045	0.89468	-1.46503
C	-11.86226	2.78616	-0.23099
H	-12.35575	3.48318	-0.91399
H	-12.04953	3.08678	0.80209
H	-12.21644	1.76103	-0.39328
C	-3.79523	-1.28195	1.17573
C	-2.38008	-1.13529	1.35978
C	-4.08356	-2.29190	0.28423
C	-1.60315	-2.00524	0.62304
S	-2.61982	-3.03924	-0.34890
C	-4.80424	-0.45009	1.90770
H	-4.46497	-0.25474	2.93065
H	-5.76800	-0.96526	1.94906
H	-4.95315	0.52028	1.41627
O	-1.82437	-0.24484	2.25217
C	-1.76547	1.11234	1.80533
C	-0.65439	1.28838	0.75831
H	-1.54567	1.71007	2.69326
H	-2.73715	1.42669	1.40657
N	-0.72030	2.63582	0.16983
H	-0.77363	0.55659	-0.04297
H	0.34095	1.17421	1.19362
C	-1.81592	3.15292	-0.40230
N	-1.53543	4.40502	-0.77961
C	-0.21777	4.68871	-0.44812
C	0.29783	3.57847	0.15279
H	1.27395	3.34486	0.57596
H	0.22692	5.64686	-0.66382
H	-2.81322	2.71422	-0.46636
C	-2.50812	5.30596	-1.39788
H	-2.30810	5.39609	-2.46911
H	-2.43077	6.28750	-0.92529
H	-3.50478	4.88939	-1.22399
C	0.63453	-2.28487	1.78007
C	2.02414	-2.24999	1.44487
C	-0.15747	-2.11963	0.66474
C	2.29431	-2.07071	0.10502
S	0.80351	-1.92287	-0.79374
C	0.13663	-2.45718	3.18273
H	-0.85004	-2.92825	3.18975
H	0.03165	-1.48676	3.68066
H	0.83449	-3.06954	3.76149
O	3.00608	-2.34980	2.40427
C	3.48963	-1.08581	2.88833
C	5.00321	-1.03363	2.64662
H	3.26478	-1.01531	3.95947
H	3.01336	-0.24547	2.37386

N	5.52580	0.31043	2.89154
H	5.21272	-1.28034	1.60770
H	5.54102	-1.74101	3.28430
C	5.71417	1.23084	1.93586
N	6.04938	2.38367	2.51808
C	6.00740	2.21770	3.89051
C	5.68234	0.91777	4.12886
H	5.56098	0.37099	5.04970
H	6.21647	3.03162	4.56539
H	5.65936	1.05957	0.87455
C	6.15626	3.64858	1.79335
H	6.74292	3.47631	0.88767
H	6.65921	4.37403	2.43478
H	5.14026	3.97456	1.55170
C	4.72002	-2.64537	-0.38375
C	5.89345	-1.96093	-0.84354
C	3.60784	-1.83604	-0.46926
C	5.66486	-0.68416	-1.29618
S	3.98956	-0.26394	-1.14326
H	6.37616	0.07981	-1.58024
C	4.74265	-4.03036	0.18906
H	5.20015	-4.03941	1.18585
H	5.32541	-4.70681	-0.44510
H	3.72709	-4.41982	0.28867
O	7.10152	-2.61373	-0.75460
C	8.25605	-1.82696	-0.98551
C	8.52591	-1.70761	-2.49757
H	9.08434	-2.34950	-0.49790
H	8.15947	-0.82470	-0.54936
N	9.56513	-0.70379	-2.74343
H	7.62006	-1.38904	-3.01536
H	8.85023	-2.65877	-2.92569
C	9.32454	0.59843	-2.95005
N	10.48855	1.25770	-2.91775
C	11.50038	0.35629	-2.62923
C	10.92520	-0.87193	-2.51764
H	11.35136	-1.84122	-2.31508
H	12.52823	0.66856	-2.53922
H	8.35817	1.04377	-3.10712
C	10.58836	2.71846	-2.92090
H	10.24769	3.11399	-3.88017
H	11.63146	2.99353	-2.76419
H	9.95826	3.08739	-2.10436
Cl	-11.58145	-0.66878	-0.90232
Cl	-4.93687	3.01950	0.01569
Cl	2.90332	2.14440	1.64901
Cl	8.08842	1.83901	-0.64766

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80.log Energy: -3690940.0238810 Ha

C	-7.32048	-2.40695	3.03920
C	-6.28610	-2.05829	2.10543
C	-7.25828	-1.60360	4.14464
C	-5.49060	-1.00395	2.48646
S	-5.98039	-0.42817	4.06519
H	-7.90393	-1.63491	5.01220
C	-8.30263	-3.51809	2.80575
H	-8.99967	-3.28556	1.99000
H	-8.88983	-3.71405	3.70768
H	-7.77854	-4.44131	2.53051
O	-6.05782	-2.77264	0.95246
C	-6.86950	-2.38379	-0.15435
C	-6.70746	-3.49912	-1.18464

H	-6.51821	-1.42652	-0.56085
H	-7.92678	-2.29421	0.11664
N	-7.59062	-3.27061	-2.32627
H	-6.98601	-4.45137	-0.73006
H	-5.67423	-3.57026	-1.53568
C	-8.79271	-3.85149	-2.47474
N	-9.41445	-3.27706	-3.51837
C	-8.63554	-2.21704	-3.96418
C	-7.49643	-2.21253	-3.22493
H	-6.62877	-1.57390	-3.25861
H	-8.96105	-1.57718	-4.76824
H	-9.12962	-4.72557	-1.94949
C	-10.82753	-3.49521	-3.81370
H	-11.00143	-4.54969	-4.04023
H	-11.10115	-2.89055	-4.67916
H	-11.39532	-3.20079	-2.92374
C	-4.39044	0.48086	0.73089
C	-3.06962	0.76555	0.25160
C	-4.36245	-0.44112	1.75203
C	-2.05645	0.11744	0.91695
S	-2.72296	-0.92400	2.15191
C	-5.61822	1.15068	0.18872
H	-5.61412	2.22572	0.41481
H	-6.52110	0.71822	0.62634
H	-5.67052	1.04509	-0.90255
O	-2.84656	1.58750	-0.83016
C	-2.66915	2.96361	-0.49384
C	-2.95719	3.74718	-1.77307
H	-1.63884	3.13652	-0.15728
H	-3.36598	3.28925	0.28558
N	-2.94394	5.18302	-1.50064
H	-3.95282	3.48544	-2.13490
H	-2.22953	3.51963	-2.55741
C	-4.05326	5.91447	-1.29464
N	-3.68303	7.13243	-0.86306
C	-2.30855	7.12756	-0.66163
C	-1.84483	5.91561	-1.06079
H	-0.84614	5.51147	-1.08917
H	-1.79349	7.98790	-0.26597
H	-5.04589	5.63358	-1.59316
C	-4.63208	8.09826	-0.31649
H	-5.36698	8.36847	-1.07819
H	-4.08555	8.99096	-0.01025
H	-5.12960	7.62269	0.53608
C	0.25386	1.16528	1.11833
C	1.60033	0.92400	0.67422
C	-0.62196	0.21191	0.66046
C	1.74944	-0.20093	-0.11499
S	0.19224	-1.00548	-0.29042
C	-0.10072	2.30936	2.02104
H	-1.16352	2.29013	2.27289
H	0.13001	3.27562	1.55577
H	0.48008	2.26268	2.94919
O	2.51947	1.84586	1.09864
C	3.91436	1.62754	0.93299
C	4.34586	2.19241	-0.42546
H	4.18226	0.57719	1.02338
H	4.39228	2.16451	1.75556
N	5.72768	1.83391	-0.75945
H	4.23923	3.28176	-0.43716
H	3.71544	1.77278	-1.20892
C	6.75055	1.76369	0.10611
N	7.84164	1.38973	-0.57023

C	7.51981	1.21046	-1.90610
C	6.19157	1.49152	-2.02425
H	5.52689	1.44678	-2.87015
H	8.25736	0.82196	-2.59939
H	6.69957	1.84197	1.18391
C	9.15120	1.14936	0.04257
H	9.69219	2.09529	0.13399
H	9.69728	0.46719	-0.61524
H	8.97490	0.71166	1.02791
C	3.87344	-1.62406	-0.14253
C	4.86897	-2.04610	-1.09225
C	2.91673	-0.83049	-0.72915
C	4.65552	-1.60683	-2.36872
S	3.21732	-0.64125	-2.46226
H	5.26175	-1.80964	-3.24041
C	3.90894	-2.02322	1.30156
H	2.97382	-1.75480	1.80005
H	4.73964	-1.53573	1.83092
H	4.05595	-3.10541	1.38878
O	5.92167	-2.84055	-0.71805
C	7.11076	-2.10940	-0.37984
C	7.81540	-2.94203	0.68641
H	6.85911	-1.13789	0.05282
H	7.73614	-1.96824	-1.27056
N	9.18149	-2.45342	0.91542
H	7.86451	-3.99002	0.37868
H	7.27942	-2.85777	1.63144
C	10.15584	-2.46672	-0.00470
N	11.23807	-1.88347	0.52230
C	10.94144	-1.48194	1.81808
C	9.64733	-1.83200	2.06384
H	8.98039	-1.61935	2.88656
H	11.66724	-0.97634	2.43407
H	10.06450	-2.77447	-1.03646
C	12.46857	-1.62201	-0.22605
H	13.11471	-2.50353	-0.21565
H	12.98548	-0.78445	0.24446
H	12.17857	-1.35708	-1.24864
Cl	-10.35699	-3.00390	-0.45098
Cl	-5.22178	4.93039	0.89824
Cl	6.87882	-0.12012	2.59309
Cl	10.02185	-0.94129	-2.66635

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90.log Energy: -3690940.0825468 Ha

C	-7.32976	2.36593	-3.11076
C	-6.25681	2.04626	-2.21225
C	-7.40861	1.43546	-4.11065
C	-5.56992	0.89446	-2.51128
S	-6.21807	0.17589	-3.96951
H	-8.11498	1.41441	-4.92987
C	-8.21658	3.56483	-2.93877
H	-8.83577	3.48673	-2.03538
H	-8.88263	3.68305	-3.79845
H	-7.61626	4.47709	-2.84080
O	-5.91647	2.85105	-1.14998
C	-6.61467	2.52980	0.05304
C	-6.27235	3.64594	1.03655
H	-6.27743	1.55741	0.43554
H	-7.69937	2.50726	-0.09859
N	-7.07839	3.50896	2.24863
H	-6.51182	4.60859	0.58166
H	-5.21183	3.63826	1.30282

C	-8.20946	4.19609	2.47788
N	-8.80767	3.67770	3.56328
C	-8.09640	2.55315	3.96182
C	-7.01601	2.44714	3.14583
H	-6.20893	1.73295	3.12309
H	-8.42069	1.94505	4.79066
H	-8.50871	5.09122	1.96550
C	-10.17281	4.02006	3.95228
H	-10.23610	5.08438	4.19021
H	-10.44163	3.43660	4.83361
H	-10.82208	3.78282	3.10194
C	-4.48674	-0.58175	-0.73745
C	-3.17046	-0.86300	-0.24602
C	-4.44784	0.32826	-1.76951
C	-2.15114	-0.22140	-0.90775
S	-2.80451	0.80951	-2.15762
C	-5.72326	-1.22759	-0.18552
H	-5.73032	-2.30870	-0.37835
H	-6.61944	-0.79389	-0.63612
H	-5.77765	-1.09617	0.90236
O	-2.94970	-1.69142	0.83038
C	-2.71134	-3.05070	0.46198
C	-2.74813	-3.84611	1.76438
H	-1.72946	-3.14044	-0.02064
H	-3.48796	-3.43111	-0.21005
N	-2.68112	-5.27778	1.47853
H	-3.69356	-3.65132	2.27317
H	-1.92619	-3.56764	2.43005
C	-3.75575	-6.08593	1.45376
N	-3.38205	-7.27078	0.94026
C	-2.06676	-7.16570	0.50512
C	-1.62618	-5.92670	0.84234
H	-0.66904	-5.45086	0.70439
H	-1.56946	-7.98416	0.01031
H	-4.69666	-5.88150	1.92917
C	-4.34227	-8.29821	0.54762
H	-4.90931	-8.63007	1.42040
H	-3.79727	-9.14504	0.12896
H	-5.01572	-7.85224	-0.19259
C	0.16577	-1.22529	-1.20689
C	1.49924	-1.05662	-0.69847
C	-0.72056	-0.34294	-0.63904
C	1.62526	-0.06895	0.25933
S	0.06834	0.71436	0.50507
C	-0.17454	-2.23917	-2.25837
H	-1.23333	-2.18325	-2.52180
H	0.04581	-3.25840	-1.91742
H	0.42100	-2.07496	-3.16345
O	2.44065	-1.90108	-1.22411
C	3.82592	-1.57126	-1.17097
C	4.45833	-2.38404	-0.03616
H	3.99102	-0.50513	-1.03289
H	4.24291	-1.84983	-2.14224
N	5.84018	-1.98242	0.24222
H	4.43078	-3.45268	-0.27160
H	3.89320	-2.21531	0.87989
C	6.76397	-1.65611	-0.67391
N	7.89092	-1.33271	-0.03097
C	7.69338	-1.44848	1.33602
C	6.40465	-1.85696	1.50641
H	5.82740	-2.03893	2.39686
H	8.47209	-1.14590	2.02812
H	6.60815	-1.53203	-1.73576

C	9.10853	-0.85082	-0.68915
H	9.68205	-1.70086	-1.06873
H	9.69071	-0.31037	0.06244
H	8.79888	-0.19956	-1.51017
C	3.67190	1.41603	0.61235
C	4.70363	1.60950	1.59662
C	2.78383	0.43846	0.99245
C	4.58235	0.81834	2.70476
S	3.19109	-0.21160	2.58588
H	5.22799	0.80441	3.57158
C	3.61485	2.18953	-0.66953
H	2.64108	2.07119	-1.15163
H	4.39228	1.85331	-1.37032
H	3.78518	3.25377	-0.47357
O	5.70153	2.53241	1.41876
C	6.87216	2.01777	0.76233
C	7.37298	3.14218	-0.14066
H	6.62242	1.15771	0.13678
H	7.62148	1.72678	1.50917
N	8.72933	2.86419	-0.63149
H	7.38503	4.08852	0.40680
H	6.72672	3.22791	-1.01379
C	9.81067	2.74549	0.15181
N	10.85592	2.43208	-0.62157
C	10.42573	2.34547	-1.93899
C	9.08862	2.60888	-1.94589
H	8.34129	2.54630	-2.72278
H	11.10123	2.09221	-2.73986
H	9.83152	2.76821	1.23236
C	12.19020	2.12428	-0.10409
H	12.76418	3.04354	0.03796
H	12.69920	1.48338	-0.82545
H	12.05781	1.59123	0.84360
Cl	-9.98575	3.51692	0.55026
Cl	-5.36497	-5.15646	-0.45998
Cl	6.45320	0.75755	-2.58936
Cl	10.16418	0.62786	2.35164

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100.log Energy: -3690940.0178192 Ha

C	-7.19400	-2.44436	3.09576
C	-6.08101	-2.07971	2.26717
C	-7.54166	-1.40315	3.91271
C	-5.62717	-0.79321	2.43101
S	-6.55493	0.01035	3.67858
H	-8.34217	-1.38113	4.64022
C	-7.85906	-3.78836	3.03007
H	-8.33752	-3.95501	2.05594
H	-8.62387	-3.88317	3.80643
H	-7.12478	-4.59036	3.17040
O	-5.50160	-2.95701	1.38026
C	-6.05328	-2.86820	0.06594
C	-5.39704	-3.99144	-0.73269
H	-5.82050	-1.88887	-0.37337
H	-7.13823	-3.02120	0.07264
N	-6.05591	-4.12854	-2.03101
H	-5.52284	-4.93179	-0.19344
H	-4.32889	-3.81295	-0.88321
C	-7.01375	-5.03348	-2.29045
N	-7.56019	-4.74261	-3.48239
C	-7.01138	-3.55096	-3.93834
C	-6.07123	-3.16696	-3.03658
H	-5.40856	-2.31705	-3.01748

H	-7.33422	-3.09820	-4.86174
H	-7.21575	-5.91096	-1.70506
C	-8.78743	-5.37168	-3.96333
H	-8.62740	-6.44339	-4.10257
H	-9.06011	-4.92051	-4.91801
H	-9.55953	-5.19790	-3.20504
C	-4.58354	0.71376	0.65667
C	-3.27139	1.08186	0.21598
C	-4.52216	-0.16366	1.71631
C	-2.23648	0.53984	0.94030
S	-2.86603	-0.51218	2.18539
C	-5.83883	1.22958	0.01741
H	-5.97388	2.30374	0.20095
H	-6.71459	0.70136	0.40280
H	-5.79783	1.09706	-1.07041
O	-3.05982	1.89410	-0.87379
C	-2.94593	3.27736	-0.53423
C	-2.87999	4.02053	-1.86630
H	-2.03317	3.44360	0.05439
H	-3.81816	3.62880	0.02793
N	-2.99642	5.46059	-1.64766
H	-3.72292	3.70862	-2.48529
H	-1.95218	3.80735	-2.40453
C	-4.14333	6.14729	-1.78908
N	-3.95547	7.38815	-1.30836
C	-2.69463	7.44827	-0.72850
C	-2.09326	6.24972	-0.94145
H	-1.11355	5.88846	-0.67449
H	-2.34372	8.33890	-0.23289
H	-5.00259	5.81427	-2.34053
C	-5.05444	8.32380	-1.08660
H	-5.54311	8.55500	-2.03588
H	-4.65122	9.24112	-0.65613
H	-5.76287	7.84088	-0.40432
C	0.08569	1.47462	1.41536
C	1.41928	1.37352	0.89250
C	-0.80950	0.72189	0.69364
C	1.53673	0.57343	-0.22656
S	-0.02570	-0.13069	-0.61566
C	-0.25139	2.30395	2.61856
H	-1.32093	2.25405	2.83557
H	0.02710	3.35350	2.46584
H	0.29880	1.95629	3.50046
O	2.38807	2.08791	1.54809
C	3.73445	1.61174	1.57165
C	4.57987	2.62279	0.79073
H	3.82683	0.61413	1.14724
H	4.03746	1.55956	2.62164
N	5.93297	2.13524	0.50894
H	4.64090	3.57312	1.33038
H	4.10541	2.80128	-0.17358
C	6.71710	1.44613	1.35094
N	7.86579	1.17570	0.72138
C	7.82498	1.69838	-0.56147
C	6.61002	2.30083	-0.69364
H	6.15073	2.80185	-1.52886
H	8.63753	1.50827	-1.25515
H	6.44071	1.05143	2.31776
C	8.95480	0.37715	1.29075
H	9.56708	1.00419	1.94459
H	9.55569	0.00788	0.45527
H	8.49823	-0.43839	1.85727
C	3.48977	-0.90429	-0.93451

C	4.58723	-0.86503	-1.86442
C	2.70261	0.21790	-1.03157
C	4.61292	0.24549	-2.66139
S	3.28443	1.30229	-2.29968
H	5.33126	0.47869	-3.43463
C	3.28708	-2.02437	0.03991
H	2.28413	-1.98947	0.47199
H	4.01848	-1.96544	0.85814
H	3.42208	-2.98929	-0.46085
O	5.51013	-1.87642	-1.92968
C	6.65168	-1.69422	-1.07461
C	6.97471	-3.07526	-0.50936
H	6.41483	-1.02746	-0.24192
H	7.48818	-1.28228	-1.65286
N	8.29455	-3.08983	0.13508
H	6.96648	-3.82156	-1.30832
H	6.24207	-3.34036	0.25230
C	9.45179	-2.86166	-0.50171
N	10.43899	-2.88983	0.40033
C	9.89292	-3.14331	1.65151
C	8.54505	-3.26126	1.48785
H	7.73487	-3.35292	2.19553
H	10.50608	-3.20060	2.53616
H	9.57477	-2.57161	-1.53620
C	11.83654	-2.58464	0.08965
H	12.35548	-3.48443	-0.25063
H	12.31524	-2.20611	0.99401
H	11.83734	-1.81075	-0.68546
Cl	-9.10416	-4.52146	-0.63604
Cl	-5.86979	5.15572	0.00707
Cl	6.02042	-1.37480	2.43474
Cl	10.18110	-0.26834	-1.98389

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cl_120.log Energy: -3690941.5774877 Ha

C	-7.06827	-2.88987	2.59253
C	-5.88554	-2.38076	1.96623
C	-7.92973	-1.86801	2.88862
C	-5.87689	-1.02235	1.74236
S	-7.33433	-0.30829	2.40123
H	-8.90460	-1.94598	3.35135
C	-7.29223	-4.35307	2.84172
H	-7.31308	-4.91888	1.90112
H	-8.23827	-4.52029	3.36471
H	-6.48267	-4.77149	3.45122
O	-4.82827	-3.19525	1.63437
C	-4.80241	-3.56294	0.25406
C	-3.59899	-4.49042	0.10491
H	-4.68730	-2.66825	-0.37222
H	-5.71263	-4.10355	-0.02866
N	-3.63883	-5.14975	-1.19980
H	-3.65216	-5.26427	0.87246
H	-2.65332	-3.95258	0.21252
C	-4.14643	-6.37661	-1.40013
N	-4.25011	-6.58155	-2.72320
C	-3.89862	-5.40879	-3.37903
C	-3.51450	-4.51465	-2.43129
H	-3.15656	-3.50103	-2.51191
H	-3.94504	-5.32717	-4.45285
H	-4.32962	-7.10807	-0.63539
C	-4.98138	-7.71016	-3.29313
H	-4.48729	-8.64800	-3.02849
H	-4.99657	-7.60353	-4.37834

H	-5.99477	-7.68239	-2.87631
C	-4.84556	0.65095	0.10872
C	-3.56195	1.23115	-0.13442
C	-4.79645	-0.24598	1.15614
C	-2.56172	0.84315	0.72913
S	-3.18504	-0.34149	1.85671
C	-6.05480	0.99981	-0.70810
H	-6.42446	2.00557	-0.46692
H	-6.86346	0.28517	-0.53849
H	-5.80096	1.00043	-1.77417
O	-3.33695	2.08712	-1.18788
C	-3.45809	3.46587	-0.82976
C	-3.40219	4.23754	-2.14598
H	-2.63007	3.75468	-0.16773
H	-4.41495	3.66769	-0.33562
N	-3.74785	5.63998	-1.92204
H	-4.13885	3.81732	-2.83281
H	-2.41459	4.17675	-2.61136
C	-4.97778	6.14682	-2.11222
N	-5.00460	7.39221	-1.60926
C	-3.79347	7.63650	-0.97489
C	-3.00677	6.54704	-1.17068
H	-1.99533	6.33536	-0.86408
H	-3.60464	8.56313	-0.45752
H	-5.75601	5.68951	-2.69416
C	-6.24292	8.14546	-1.42965
H	-6.71152	8.32846	-2.39937
H	-6.00587	9.09953	-0.95758
H	-6.90264	7.54012	-0.79777
C	-0.31729	1.61506	1.66757
C	1.03477	1.75284	1.21785
C	-1.15369	1.19617	0.65505
C	1.23534	1.46087	-0.11557
S	-0.27280	0.94939	-0.84457
C	-0.72602	1.89906	3.08359
H	-1.81207	1.97425	3.17230
H	-0.27514	2.83319	3.43418
H	-0.38738	1.10556	3.76131
O	1.99291	2.19033	2.09917
C	3.21468	1.44510	2.17329
C	4.30451	2.47999	2.46513
H	3.43685	0.92352	1.24351
H	3.13569	0.69130	2.96443
N	5.63942	1.99328	2.10809
H	4.29997	2.79265	3.51345
H	4.11109	3.35429	1.84372
C	6.19749	0.84828	2.52575
N	7.39307	0.72792	1.93966
C	7.60864	1.81292	1.10486
C	6.50574	2.60574	1.21034
H	6.24407	3.53003	0.72372
H	8.49832	1.85618	0.48444
H	5.73353	0.10190	3.14922
C	8.27570	-0.43155	2.08648
H	8.79526	-0.38007	3.04722
H	8.99744	-0.39623	1.26578
H	7.64847	-1.32431	2.03140
C	3.21601	0.47236	-1.38324
C	4.48342	0.92041	-1.89454
C	2.48111	1.51539	-0.86851
C	4.69320	2.26708	-1.78513
S	3.33786	3.04997	-1.03743
H	5.55992	2.82150	-2.11612

C	2.83457	-0.97630	-1.33586
H	1.76462	-1.10079	-1.15783
H	3.37711	-1.47581	-0.52135
H	3.09614	-1.46945	-2.27819
O	5.39478	0.04502	-2.42753
C	6.36627	-0.44754	-1.48686
C	6.45391	-1.95416	-1.72133
H	6.03704	-0.27401	-0.45981
H	7.33082	0.04612	-1.65541
N	7.59151	-2.54202	-1.00200
H	6.56830	-2.16536	-2.78802
H	5.55302	-2.43853	-1.34661
C	8.87801	-2.27302	-1.26321
N	9.63344	-2.93276	-0.37828
C	8.79967	-3.63587	0.48118
C	7.51679	-3.38571	0.09587
H	6.56372	-3.63314	0.54011
H	9.19306	-4.23223	1.28828
H	9.25133	-1.56619	-1.98810
C	11.08655	-2.78898	-0.27980
H	11.58235	-3.41851	-1.02305
H	11.39472	-3.09465	0.72093
H	11.32059	-1.73061	-0.43928
Cl	-6.77485	-6.34764	-0.67161
Cl	-6.65491	4.87924	-0.41361
Cl	5.00186	-1.79588	1.52952
Cl	10.05254	0.50581	-0.84914

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c1_140.log	Energy: -3690953.7499917 Ha		
C	6.51479	-4.92975	-0.22131
C	5.47990	-3.94961	-0.33630
C	7.71829	-4.33840	0.05425
C	5.88601	-2.64389	-0.11708
S	7.61421	-2.61008	0.18518
H	8.67034	-4.82794	0.21061
C	6.25501	-6.39778	-0.39347
H	5.43197	-6.73048	0.24867
H	7.14508	-6.98645	-0.15397
H	5.95978	-6.62348	-1.42484
O	4.21909	-4.31069	-0.72611
C	3.15239	-4.16185	0.22722
C	1.88188	-4.30753	-0.60681
H	3.19826	-3.17816	0.70568
H	3.19115	-4.95778	0.97787
N	0.71443	-3.71011	0.05421
H	1.67095	-5.36837	-0.75677
H	2.01190	-3.79447	-1.56080
C	-0.05831	-4.35048	0.94240
N	-1.04398	-3.51562	1.29993
C	-0.89688	-2.30851	0.62981
C	0.21574	-2.42999	-0.14948
H	0.69417	-1.72792	-0.81395
H	-1.62788	-1.52172	0.73814
H	0.16674	-5.38510	1.27635
C	-2.08668	-3.82646	2.27793
H	-2.16019	-4.91081	2.36867
H	-3.02740	-3.39419	1.92950
H	-1.82068	-3.39703	3.24794
C	5.09826	-0.29103	0.53453
C	4.05449	0.59838	0.14510
C	5.06534	-1.45617	-0.21109
C	3.25178	0.17820	-0.89791

S	3.80159	-1.39680	-1.43886
C	6.03513	0.03400	1.66020
H	6.84368	0.69994	1.33062
H	6.47883	-0.86939	2.08450
H	5.49159	0.56313	2.45005
O	3.77429	1.74105	0.85795
C	4.44313	2.90645	0.36198
C	4.23014	3.98330	1.42329
H	4.00507	3.20744	-0.59932
H	5.51710	2.72735	0.23957
N	5.06988	5.14476	1.13826
H	4.52535	3.58653	2.39628
H	3.18466	4.29878	1.47897
C	6.28876	5.33664	1.67089
N	6.86411	6.37670	1.04614
C	6.03468	6.78067	0.00835
C	4.91390	6.01560	0.06426
H	4.02103	6.01626	-0.53963
H	6.31530	7.57801	-0.66058
H	6.67559	4.83324	2.53734
C	8.27528	6.71678	1.20979
H	8.47356	6.99270	2.24798
H	8.50808	7.56166	0.56080
H	8.85688	5.82960	0.93487
C	1.16542	0.39952	-2.34867
C	-0.16785	0.88451	-2.19869
C	1.94981	0.70236	-1.24621
C	-0.41787	1.57905	-1.03252
S	1.01843	1.58584	-0.03232
C	1.59770	-0.38047	-3.55844
H	2.65111	-0.20477	-3.79294
H	0.99165	-0.09526	-4.42261
H	1.47228	-1.46251	-3.41681
O	-1.12675	0.63948	-3.15934
C	-2.20829	-0.18298	-2.70154
C	-3.34079	-0.00607	-3.72127
H	-2.54830	0.13212	-1.71195
H	-1.87499	-1.22592	-2.63229
N	-4.65659	0.11341	-3.08345
H	-3.37727	-0.82019	-4.44998
H	-3.16369	0.92663	-4.25666
C	-5.20521	-0.77576	-2.24204
N	-6.40394	-0.31514	-1.87160
C	-6.63141	0.91258	-2.47012
C	-5.53238	1.18037	-3.23125
H	-5.28184	2.02969	-3.84496
H	-7.52504	1.47912	-2.22853
H	-4.73638	-1.66412	-1.84720
C	-7.32436	-1.00860	-0.96574
H	-7.89264	-1.75464	-1.52824
H	-8.00096	-0.25482	-0.55396
H	-6.72267	-1.48101	-0.18786
C	-2.36951	2.03998	0.55904
C	-3.66843	2.64802	0.48339
C	-1.67399	2.18160	-0.62379
C	-3.95305	3.23763	-0.71642
S	-2.62665	3.07230	-1.81892
H	-4.86292	3.74705	-1.00061
C	-1.94697	1.26618	1.77180
H	-0.96504	0.80863	1.64032
H	-2.67699	0.47159	1.96410
H	-1.90793	1.91186	2.65659
O	-4.53113	2.56947	1.54463

C	-5.69500	1.76722	1.30106
C	-5.98142	1.06616	2.62521
H	-5.47833	1.01039	0.54448
H	-6.53792	2.38353	0.96852
N	-7.19625	0.24707	2.53536
H	-6.10197	1.79185	3.43402
H	-5.15656	0.39300	2.85653
C	-8.43170	0.72511	2.33500
N	-9.27251	-0.31022	2.23113
C	-8.54501	-1.48653	2.34781
C	-7.24086	-1.13868	2.53376
H	-6.33300	-1.72098	2.58299
H	-9.01834	-2.45271	2.28129
H	-8.70075	1.75950	2.19749
C	-10.68488	-0.17760	1.86909
H	-11.26075	0.19105	2.72130
H	-11.05754	-1.15948	1.57569
H	-10.74095	0.52034	1.02638
Cl	1.42816	-7.05935	1.29452
Cl	7.89414	3.31862	0.83118
Cl	-4.30933	-1.47810	0.78231
Cl	-9.03688	1.99618	-0.33235

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cl_180.log	Energy: -3690931.7221064 Ha		
C	8.14830	1.55630	-0.22976
C	6.75839	1.25670	-0.38333
C	8.30945	2.76213	0.39698
C	5.87982	2.20668	0.11444
S	6.80832	3.53341	0.80173
H	9.24080	3.25303	0.64519
C	9.25126	0.65627	-0.70646
H	9.38558	-0.21720	-0.05322
H	10.20162	1.19662	-0.74524
H	9.02868	0.27900	-1.71120
O	6.30987	0.12583	-1.02617
C	6.33070	-1.06350	-0.22460
C	5.84943	-2.17539	-1.15243
H	5.64545	-0.95824	0.62528
H	7.33892	-1.27231	0.15297
N	5.76269	-3.44060	-0.42059
H	6.53737	-2.28809	-1.99408
H	4.85641	-1.94584	-1.54204
C	6.80686	-3.99319	0.21393
N	6.35694	-5.06435	0.87743
C	4.99334	-5.20759	0.65436
C	4.61863	-4.18208	-0.15903
H	3.64142	-3.95227	-0.55336
H	4.39274	-5.99743	1.07511
H	7.83453	-3.57584	0.30735
C	7.21707	-5.88234	1.73124
H	8.16211	-5.34768	1.85890
H	7.39161	-6.85694	1.26773
H	6.73522	-6.01732	2.70204
C	3.51771	3.03212	0.68290
C	2.18319	2.56853	0.51157
C	4.43764	2.15322	0.12557
C	2.03747	1.35538	-0.13945
S	3.62494	0.76348	-0.59878
C	3.81986	4.30676	1.41785
H	4.16193	5.10421	0.74844
H	4.58631	4.15406	2.18453
H	2.91823	4.67252	1.91347

O	1.09314	3.25872	0.99235
C	0.68613	4.34763	0.15210
C	-0.51259	4.97124	0.86114
H	0.39814	3.96738	-0.83656
H	1.47822	5.09468	0.03837
N	-0.97656	6.15027	0.13537
H	-0.21977	5.28510	1.86490
H	-1.33495	4.25606	0.94668
C	-0.61451	7.41150	0.42974
N	-1.06499	8.21782	-0.54808
C	-1.60494	7.42742	-1.55535
C	-1.55451	6.13903	-1.13098
H	-1.88110	5.22244	-1.59507
H	-1.98145	7.85781	-2.46911
H	-0.20936	7.73657	1.36973
C	-0.65112	9.61201	-0.67246
H	-0.98560	10.17920	0.19946
H	-1.10393	10.03252	-1.57116
H	0.44307	9.62306	-0.73420
C	0.63260	-0.57970	-1.05542
C	-0.74310	-0.93725	-1.12167
C	0.82037	0.64078	-0.41931
C	-1.63430	-0.03154	-0.57287
S	-0.72780	1.32358	0.08574
C	1.70267	-1.46623	-1.62639
H	2.33758	-0.92766	-2.33831
H	1.24701	-2.30794	-2.15277
H	2.35004	-1.87159	-0.83953
O	-1.16337	-2.11151	-1.71007
C	-1.11460	-3.24300	-0.83365
C	-1.74250	-4.38694	-1.62579
H	-1.70048	-3.04078	0.07126
H	-0.08860	-3.49769	-0.54495
N	-1.82937	-5.58427	-0.79078
H	-1.13477	-4.62431	-2.50089
H	-2.74599	-4.11664	-1.95955
C	-0.91409	-6.56059	-0.76184
N	-1.20524	-7.38486	0.25266
C	-2.31076	-6.88514	0.92626
C	-2.70389	-5.75801	0.27481
H	-3.51610	-5.07195	0.45565
H	-2.71596	-7.38045	1.79368
H	-0.08012	-6.66066	-1.43327
C	-0.30430	-8.44222	0.70925
H	-0.22195	-9.22048	-0.05287
H	-0.71127	-8.87270	1.62451
H	0.67102	-7.97872	0.89357
C	-3.97777	0.73411	0.11728
C	-5.32246	0.24385	0.02328
C	-3.07145	-0.12981	-0.47911
C	-5.45564	-0.95751	-0.61896
S	-3.91070	-1.52608	-1.16751
H	-6.35343	-1.52778	-0.82532
C	-3.66874	2.03630	0.80171
H	-2.97752	1.90417	1.64224
H	-4.59090	2.47798	1.18620
H	-3.20940	2.75760	0.11370
O	-6.33711	0.98553	0.57283
C	-7.59967	0.34079	0.52821
C	-8.63751	1.34151	1.02312
H	-7.60321	-0.55907	1.15580
H	-7.84600	0.01044	-0.48468
N	-9.93996	0.67991	1.14758

H	-8.72838	2.18730	0.33610
H	-8.36899	1.73201	2.00731
C	-10.64067	0.16777	0.12135
N	-11.70329	-0.48186	0.61725
C	-11.62498	-0.46643	2.00111
C	-10.52497	0.25844	2.33516
H	-10.11304	0.52632	3.29448
H	-12.35929	-0.96305	2.61429
H	-10.42126	0.30351	-0.92233
C	-12.55921	-1.34827	-0.19232
H	-13.04724	-0.76161	-0.97354
H	-13.31635	-1.79087	0.45553
H	-11.90983	-2.11235	-0.63668
Cl	9.45784	-2.67604	1.11630
Cl	2.01891	7.58959	0.05799
Cl	1.59944	-5.55787	0.10298
Cl	-9.33040	-2.07919	-0.95339

8.4 Coordinates of optimized structures

geometries optimized at the B3LYP-D3(BJ)/6-31G(d) level

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C₁ ($\bar{\theta} = 8^\circ$) CPT conformer Energy: -3690932.0224324 Ha

C	8.24678	1.00435	-0.12105
C	6.84041	0.80110	-0.27800
C	8.49188	2.23561	0.42417
C	6.03083	1.84056	0.15150
S	7.04843	3.14330	0.75122
H	9.45462	2.66978	0.65796
C	9.28005	-0.01049	-0.51507
H	9.31208	-0.85942	0.18211
H	10.27587	0.44133	-0.54372
H	9.05684	-0.41611	-1.50862
O	6.31636	-0.32129	-0.87556
C	6.17955	-1.45880	-0.01226
C	5.65513	-2.57131	-0.91534
H	5.45587	-1.24473	0.78389
H	7.14104	-1.73463	0.43800
N	5.40359	-3.78657	-0.13823
H	6.38088	-2.78766	-1.70331
H	4.71396	-2.27334	-1.38038
C	6.34214	-4.39444	0.60176
N	5.75475	-5.41198	1.24230
C	4.40995	-5.46267	0.89682
C	4.18871	-4.43585	0.03073
H	3.27103	-4.14878	-0.45862
H	3.71758	-6.19711	1.27476
H	7.39425	-4.05732	0.75635
C	6.47019	-6.27566	2.17953
H	7.45881	-5.84068	2.34507
H	6.56594	-7.28265	1.76501
H	5.92257	-6.31708	3.12379
C	3.72525	2.83590	0.67596
C	2.36513	2.49038	0.44195
C	4.58922	1.89805	0.12626
C	2.14430	1.31851	-0.25949
S	3.69314	0.60625	-0.67900
C	4.09957	4.06319	1.45650
H	4.44142	4.88049	0.81047
H	4.88774	3.85030	2.18495
H	3.22686	4.43339	1.99998
O	1.31862	3.25180	0.91284

C	1.01657	4.37329	0.07184
C	-0.12652	5.10850	0.76496
H	0.70569	4.02097	-0.92047
H	1.87457	5.04523	-0.03294
N	-0.46316	6.32258	0.02573
H	0.18161	5.39898	1.77115
H	-1.01565	4.47655	0.84158
C	0.02130	7.54331	0.31428
N	-0.32953	8.38085	-0.67731
C	-0.93701	7.64044	-1.68383
C	-1.02487	6.35806	-1.24752
H	-1.43952	5.47545	-1.70707
H	-1.25667	8.09824	-2.60591
H	0.45835	7.83202	1.25185
C	0.23108	9.72190	-0.81384
H	-0.02881	10.32407	0.05983
H	-0.18613	10.18562	-1.70852
H	1.31923	9.61422	-0.88770
C	0.61366	-0.45185	-1.29593
C	-0.77771	-0.74518	-1.32737
C	0.88232	0.70280	-0.57277
C	-1.60209	0.14108	-0.65754
S	-0.61190	1.40776	0.05459
C	1.61382	-1.34041	-1.97850
H	2.31163	-0.76822	-2.59819
H	1.09207	-2.05277	-2.62245
H	2.20474	-1.91408	-1.25321
O	-1.27132	-1.84517	-1.99674
C	-1.32005	-3.02649	-1.18936
C	-2.01578	-4.07502	-2.05364
H	-1.90700	-2.83656	-0.28276
H	-0.32058	-3.36756	-0.89690
N	-2.27194	-5.28077	-1.26651
H	-1.39498	-4.34827	-2.90910
H	-2.96863	-3.69009	-2.42179
C	-1.44395	-6.32922	-1.18341
N	-1.89439	-7.14971	-0.22573
C	-3.01609	-6.57720	0.35696
C	-3.25453	-5.40628	-0.29251
H	-4.02154	-4.65854	-0.16606
H	-3.54071	-7.05795	1.16660
H	-0.55455	-6.47637	-1.77023
C	-1.13051	-8.29122	0.27633
H	-1.05129	-9.05919	-0.49648
H	-1.64956	-8.70128	1.14305
H	-0.13814	-7.91849	0.55317
C	-3.86926	0.84945	0.29698
C	-5.24446	0.46685	0.15423
C	-3.03809	0.09254	-0.51438
C	-5.47182	-0.55196	-0.73131
S	-3.98211	-1.06992	-1.45645
H	-6.40787	-1.02129	-1.01007
C	-3.45505	1.93745	1.24759
H	-2.65105	1.61141	1.91603
H	-4.30954	2.23850	1.85820
H	-3.09373	2.82868	0.71754
O	-6.19248	1.11632	0.90365
C	-7.48421	0.53927	0.80756
C	-8.44569	1.44815	1.56456
H	-7.49426	-0.47176	1.23338
H	-7.80316	0.43726	-0.23352
N	-9.77095	0.82275	1.62091
H	-8.52884	2.42468	1.07963

H	-8.11095	1.60774	2.59198
C	-10.53899	0.55744	0.55049
N	-11.60641	-0.14311	0.95864
C	-11.46849	-0.41161	2.31144
C	-10.32287	0.19000	2.72758
H	-9.85833	0.24221	3.69878
H	-12.19754	-0.99587	2.84893
H	-10.35620	0.89006	-0.45548
C	-12.53671	-0.79183	0.03509
H	-13.05332	-0.03782	-0.56272
H	-13.26587	-1.35590	0.61724
H	-11.93875	-1.44928	-0.60796
Cl	9.09004	-3.24754	1.48217
Cl	2.68049	7.46395	-0.01876
Cl	1.07149	-5.59561	-0.05654
Cl	-9.38583	-1.46083	-1.04902

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C₂ ($\bar{\theta} = 13^\circ$) CPT conformer Energy: -3690940.6535491 Ha

C	-6.02080	4.70040	-0.08513
C	-5.00448	3.72515	0.15373
C	-5.46882	5.84937	-0.58491
C	-3.71337	4.10874	-0.17451
S	-3.74596	5.76217	-0.76958
H	-5.98492	6.76048	-0.85633
C	-7.47802	4.46409	0.18872
H	-7.93360	3.79061	-0.55040
H	-8.03287	5.40673	0.17300
H	-7.61177	4.00255	1.17398
O	-5.27112	2.50687	0.73605
C	-5.75336	1.49755	-0.15890
C	-6.03835	0.29388	0.73474
H	-4.98284	1.24541	-0.89779
H	-6.65915	1.82729	-0.68219
N	-6.46910	-0.85134	-0.06956
H	-6.81663	0.54105	1.46113
H	-5.13727	0.00100	1.27597
C	-7.51257	-0.80689	-0.90985
N	-7.57078	-1.98354	-1.54461
C	-6.54535	-2.80488	-1.09312
C	-5.84929	-2.08934	-0.16705
H	-4.98576	-2.38181	0.40929
H	-6.37757	-3.80950	-1.44550
H	-8.15767	0.07530	-1.13728
C	-8.56505	-2.27505	-2.57569
H	-9.09283	-1.34448	-2.79990
H	-9.26836	-3.03124	-2.21699
H	-8.05957	-2.63883	-3.47316
C	-1.22676	3.58600	-0.52938
C	-0.33837	2.51173	-0.24276
C	-2.50935	3.32014	-0.06749
C	-0.88988	1.42006	0.40434
S	-2.58696	1.74039	0.71847
C	-0.76773	4.80729	-1.27102
H	-0.58769	5.65794	-0.59944
H	-1.49274	5.10887	-2.03298
H	0.17677	4.58784	-1.77769
O	0.98590	2.53131	-0.62106
C	1.81951	3.27229	0.28137
C	3.16593	3.44569	-0.41905
H	1.94226	2.71777	1.22025
H	1.36295	4.24491	0.50281

N	4.00685	4.35853	0.36749
H	3.01147	3.87619	-1.41181
H	3.70634	2.50268	-0.52367
C	3.64744	5.61696	0.65906
N	4.56962	6.12674	1.48180
C	5.55057	5.17129	1.71272
C	5.19589	4.05427	1.01526
H	5.66676	3.08793	0.88306
H	6.39964	5.36977	2.34697
H	2.69592	6.13600	0.42323
C	4.46277	7.46591	2.06485
H	3.43280	7.80718	1.91064
H	5.17117	8.14401	1.58134
H	4.67897	7.40537	3.13372
C	-0.75711	-0.93007	1.40694
C	0.17906	-1.99727	1.44279
C	-0.25309	0.17046	0.72154
C	1.38138	-1.77052	0.80027
S	1.38305	-0.14470	0.13754
C	-2.11459	-1.05766	2.03637
H	-2.34819	-0.20491	2.68205
H	-2.15393	-1.96701	2.64152
H	-2.90475	-1.12479	1.27782
O	-0.09372	-3.18658	2.08974
C	-0.65974	-4.17876	1.23031
C	-0.75818	-5.43956	2.08456
H	0.00032	-4.35311	0.37114
H	-1.65077	-3.88860	0.86329
N	-1.26274	-6.55486	1.28451
H	-1.44380	-5.28157	2.91908
H	0.22331	-5.70613	2.48342
C	-2.54255	-6.94682	1.23777
N	-2.66907	-7.87162	0.27581
C	-1.44598	-8.01218	-0.36418
C	-0.56427	-7.19157	0.26597
H	0.48419	-7.00406	0.09852
H	-1.31821	-8.68457	-1.19693
H	-3.32620	-6.60754	1.89044
C	-3.96265	-8.35241	-0.20558
H	-4.49747	-8.85499	0.60329
H	-3.79087	-9.05808	-1.01884
H	-4.52527	-7.47757	-0.54962
C	3.54513	-2.65296	-0.23469
C	4.49345	-3.69675	0.03280
C	2.50968	-2.66351	0.68437
C	4.19360	-4.49273	1.09924
S	2.71131	-3.98811	1.84633
H	4.75034	-5.34405	1.46347
C	3.68395	-1.73214	-1.41409
H	2.70942	-1.49213	-1.84773
H	4.28457	-2.22113	-2.18946
H	4.17572	-0.78600	-1.15237
O	5.60211	-3.91141	-0.76725
C	6.63199	-2.94619	-0.59948
C	7.42761	-2.96301	-1.90511
H	7.27820	-3.21124	0.24984
H	6.22077	-1.94648	-0.41503
N	8.50398	-1.96463	-1.87230
H	6.76514	-2.74043	-2.74459
H	7.88052	-3.94175	-2.07450
C	8.28244	-0.65022	-1.73277
N	9.46735	-0.03619	-1.65445
C	10.47728	-0.97970	-1.75574

C	9.87107	-2.19388	-1.88827
H	10.28243	-3.18507	-1.99350
H	11.52038	-0.70820	-1.72410
H	7.31843	-0.13720	-1.57196
C	9.61232	1.40981	-1.45175
H	8.63661	1.79578	-1.14152
H	9.93642	1.88435	-2.38097
H	10.35011	1.58487	-0.66643
Cl	-9.03589	1.66576	-1.99277
Cl	1.00636	7.14356	0.99210
Cl	-4.05774	-4.90422	0.07141
Cl	6.07136	1.10486	-0.47280

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C₃ ($\bar{\theta} = 16^\circ$) CPT conformer Energy: -3690957.1900174 Ha

C	-8.41501	-1.17773	0.08189
C	-7.09019	-0.97314	-0.41894
C	-8.61695	-2.49826	0.37638
C	-6.29645	-2.10651	-0.49373
S	-7.22562	-3.49198	0.06532
H	-9.51709	-2.95476	0.76506
C	-9.41476	-0.07205	0.25252
H	-9.18000	0.55559	1.12435
H	-10.42196	-0.47688	0.38692
H	-9.41789	0.57850	-0.62945
O	-6.63805	0.25321	-0.84223
C	-6.17095	1.11456	0.21035
C	-5.84026	2.43964	-0.47078
H	-5.26827	0.69075	0.66743
H	-6.93598	1.24562	0.98564
N	-5.27226	3.37878	0.49934
H	-6.74198	2.87281	-0.91082
H	-5.10353	2.29235	-1.26208
C	-5.91284	3.76039	1.61462
N	-5.07193	4.52334	2.32289
C	-3.86668	4.64130	1.64236
C	-3.99143	3.91724	0.49661
H	-3.26696	3.76245	-0.28648
H	-3.01692	5.20284	1.99674
H	-6.90042	3.39653	1.96883
C	-5.41590	5.08286	3.62831
H	-6.33366	4.59762	3.96886
H	-5.56614	6.16267	3.54832
H	-4.60643	4.87636	4.33174
C	-4.00965	-3.22831	-0.80975
C	-2.70821	-2.83873	-1.23506
C	-4.91647	-2.18128	-0.90807
C	-2.58044	-1.53294	-1.67285
S	-4.14614	-0.75076	-1.58962
C	-4.30199	-4.61529	-0.31223
H	-5.09746	-5.09388	-0.89393
H	-4.62455	-4.61831	0.73604
H	-3.40797	-5.23806	-0.40839
O	-1.63062	-3.71067	-1.18100
C	-0.95505	-3.69191	0.07177
C	0.21983	-4.66057	-0.07170
H	-1.63348	-4.01874	0.87195
H	-0.60238	-2.68179	0.31022
N	0.72911	-5.07530	1.24165
H	1.04039	-4.20807	-0.62889
H	-0.11483	-5.55281	-0.60759
C	1.93539	-4.79053	1.75872

N	2.00133	-5.34419	2.97754
C	0.81082	-5.99665	3.24594
C	0.01085	-5.82970	2.15798
H	-0.98807	-6.17880	1.95079
H	0.64442	-6.51776	4.17525
H	2.77241	-4.24303	1.30629
C	3.15928	-5.26987	3.87871
H	3.96800	-4.75938	3.34438
H	3.46099	-6.28448	4.14767
H	2.87683	-4.71375	4.77572
C	-1.16443	0.53043	-2.19413
C	0.18541	0.81357	-2.54961
C	-1.39056	-0.83565	-2.08890
C	1.00498	-0.28716	-2.70688
S	0.07310	-1.74800	-2.46523
C	-2.13857	1.63668	-1.90552
H	-2.92172	1.69880	-2.67165
H	-1.61590	2.59605	-1.87291
H	-2.62939	1.48609	-0.93850
O	0.65067	2.10005	-2.65691
C	1.32922	2.54534	-1.47437
C	1.89980	3.91588	-1.80574
H	2.13458	1.84639	-1.21881
H	0.62456	2.63645	-0.64056
N	2.79617	4.34282	-0.72701
H	1.09092	4.64300	-1.88728
H	2.47620	3.87772	-2.73203
C	2.40266	5.03325	0.35060
N	3.45748	5.13793	1.17320
C	4.54979	4.49066	0.60965
C	4.12949	3.98476	-0.58157
H	4.67153	3.40193	-1.30936
H	5.52689	4.41181	1.06529
H	1.36308	5.33719	0.52338
C	3.44311	5.83003	2.45678
H	4.08398	6.71431	2.41298
H	3.80389	5.15655	3.23745
H	2.41859	6.12980	2.68017
C	3.38525	-1.11520	-2.33191
C	4.71767	-0.68843	-2.64773
C	2.43840	-0.28783	-2.90754
C	4.78287	0.40134	-3.47136
S	3.19963	0.96790	-3.88445
H	5.67201	0.90451	-3.82366
C	3.11095	-2.30025	-1.45116
H	2.36921	-2.05824	-0.68175
H	4.01774	-2.64217	-0.94939
H	2.72173	-3.14421	-2.03593
O	5.82530	-1.29524	-2.10474
C	6.13531	-0.76789	-0.80970
C	7.26534	-1.62721	-0.25722
H	5.26952	-0.84497	-0.14107
H	6.42769	0.28801	-0.88813
N	7.70221	-1.08554	1.03640
H	8.11581	-1.63654	-0.94376
H	6.90968	-2.64377	-0.08510
C	8.24114	0.13079	1.19901
N	8.41813	0.33468	2.50886
C	7.97915	-0.78526	3.20127
C	7.51971	-1.67610	2.27752
H	7.01462	-2.62903	2.36321
H	8.02350	-0.83958	4.27700
H	8.36655	0.90587	0.44397

C	8.91848	1.58878	3.07295
H	8.67788	2.38632	2.36169
H	9.99706	1.52599	3.24023
H	8.40986	1.77050	4.02165
Cl	-8.28608	2.26440	2.97102
Cl	4.93674	-3.67199	1.42538
Cl	-0.78406	4.84017	0.26256
Cl	7.38625	2.91967	0.13199

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C₄ ($\bar{\theta} = 17^\circ$) CPT conformer Energy: -3690933.8286243 Ha

C	7.51499	-1.72921	-2.11835
C	6.24232	-1.51976	-1.50419
C	8.11457	-0.52920	-2.39212
C	5.88679	-0.19895	-1.29385
S	7.16076	0.83961	-1.91386
H	9.07793	-0.36753	-2.85695
C	8.07638	-3.09063	-2.41238
H	8.31885	-3.64491	-1.49652
H	8.98739	-3.01287	-3.01281
H	7.34921	-3.69437	-2.96771
O	5.40604	-2.56270	-1.16801
C	5.67831	-3.11249	0.12494
C	4.66707	-4.24018	0.30700
H	5.53975	-2.34239	0.89504
H	6.69406	-3.51640	0.18963
N	4.94437	-4.96096	1.54833
H	4.75448	-4.94583	-0.52119
H	3.64428	-3.85604	0.33494
C	5.69102	-6.07387	1.62426
N	5.91639	-6.34481	2.92018
C	5.38720	-5.31253	3.68402
C	4.77802	-4.44888	2.83069
H	4.23578	-3.53391	3.00686
H	5.48588	-5.29715	4.75729
H	5.96727	-6.69795	0.79492
C	6.89067	-7.33875	3.36268
H	6.58814	-8.33309	3.02610
H	6.93394	-7.32382	4.45233
H	7.85518	-7.06484	2.91941
C	4.35778	1.57128	-0.24912
C	3.01865	1.64569	0.24697
C	4.66574	0.29873	-0.70272
C	2.30235	0.46822	0.19724
S	3.29663	-0.80337	-0.48500
C	5.25424	2.77487	-0.25457
H	5.26603	3.27439	-1.23388
H	6.28171	2.51370	0.01602
H	4.88424	3.50184	0.47476
O	2.48419	2.81968	0.71973
C	1.94055	3.65710	-0.30681
C	1.64091	4.99778	0.36232
H	1.02173	3.21107	-0.70901
H	2.66403	3.77760	-1.12355
N	1.29031	5.99198	-0.65983
H	2.52952	5.34332	0.89690
H	0.80241	4.93266	1.05920
C	2.12204	6.35000	-1.64766
N	1.46127	7.18256	-2.45833
C	0.17551	7.37004	-1.96694
C	0.06360	6.61672	-0.83527
H	-0.74400	6.45141	-0.13079

H	-0.53415	8.01279	-2.46272
H	3.12215	5.93566	-1.88597
C	2.04310	7.72057	-3.68918
H	2.93450	7.12542	-3.91607
H	2.30642	8.77296	-3.55294
H	1.31591	7.62346	-4.49831
C	0.19889	0.74182	1.62295
C	-1.15302	0.29560	1.58168
C	0.92421	0.23849	0.55993
C	-1.49313	-0.54977	0.54092
S	-0.07003	-0.79614	-0.46260
C	0.72198	1.59261	2.74215
H	1.79657	1.44823	2.87213
H	0.20693	1.33276	3.67326
H	0.56055	2.65984	2.55404
O	-2.06791	0.67362	2.54269
C	-2.66832	1.93903	2.25806
C	-3.62369	2.20384	3.41716
H	-3.22671	1.88893	1.31509
H	-1.92425	2.73825	2.17734
N	-4.40658	3.41182	3.14903
H	-3.07522	2.34470	4.35083
H	-4.31418	1.36744	3.54308
C	-3.99962	4.65909	3.41394
N	-4.86741	5.51499	2.86093
C	-5.83099	4.78899	2.17712
C	-5.54303	3.47097	2.35434
H	-6.03074	2.57670	1.99975
H	-6.63020	5.27394	1.64049
H	-3.10742	4.92926	3.95158
C	-4.63973	6.95834	2.78622
H	-4.67399	7.39588	3.78642
H	-5.42321	7.39974	2.16986
H	-3.65327	7.10691	2.33315
C	-3.18409	-1.89709	-0.82629
C	-4.56969	-2.25825	-0.73844
C	-2.78202	-1.13953	0.26128
C	-5.21840	-1.79332	0.37363
S	-4.12597	-0.90641	1.38948
H	-6.25305	-1.92485	0.66707
C	-2.33405	-2.31513	-1.99290
H	-1.89284	-1.45298	-2.50623
H	-2.94193	-2.86521	-2.71472
H	-1.50683	-2.96513	-1.68402
O	-5.12287	-3.00673	-1.74592
C	-6.52487	-3.17544	-1.62523
C	-6.95642	-4.16272	-2.70355
H	-7.04726	-2.21843	-1.74715
H	-6.80088	-3.55309	-0.63668
N	-8.41990	-4.25830	-2.72417
H	-6.53324	-5.15431	-2.52160
H	-6.63210	-3.83220	-3.69275
C	-9.17239	-4.71686	-1.70972
N	-10.46230	-4.52320	-2.01851
C	-10.53143	-3.84030	-3.22256
C	-9.25718	-3.67338	-3.66541
H	-8.86833	-3.21207	-4.55857
H	-11.47512	-3.54584	-3.65210
H	-8.80761	-5.19651	-0.81924
C	-11.54923	-4.69788	-1.05574
H	-11.60423	-5.74300	-0.74351
H	-12.48595	-4.41248	-1.53531
H	-11.32109	-4.05214	-0.19874

C1	8.22928	-5.49000	0.79271
C1	4.42493	4.96983	-3.14668
C1	-1.66029	5.40432	1.87740
C1	-9.08461	-2.95955	0.50382

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C₅ ($\bar{\theta} = 43^\circ$) CPT conformer Energy: -3690972.5496232 Ha

C	-8.20650	0.22379	1.90025
C	-6.93753	0.15511	1.21989
C	-8.73403	1.48168	1.85923
C	-6.54235	1.35562	0.65672
S	-7.73398	2.60773	0.99887
H	-9.66619	1.81235	2.29785
C	-8.82107	-0.97103	2.56639
H	-8.99049	-1.77656	1.84334
H	-9.77644	-0.71312	3.03244
H	-8.15598	-1.37716	3.33747
O	-6.32378	-1.06018	1.22710
C	-4.90614	-1.20976	1.11794
C	-4.23628	-0.59592	2.35573
H	-4.52593	-0.76621	0.19879
H	-4.73031	-2.28466	1.07006
N	-2.77773	-0.74164	2.32964
H	-4.60032	-1.09603	3.25569
H	-4.46727	0.46864	2.43285
C	-2.08752	-1.64931	3.03258
N	-0.78617	-1.51078	2.75137
C	-0.64084	-0.53434	1.77744
C	-1.88678	-0.04969	1.51209
H	-2.21631	0.72971	0.84861
H	0.33978	-0.27688	1.39966
H	-2.50868	-2.35254	3.72808
C	0.24944	-2.44644	3.19104
H	0.24548	-2.50464	4.28234
H	1.21389	-2.07421	2.84104
H	0.00475	-3.42325	2.76180
C	-5.03261	1.10305	-1.36476
C	-3.68174	1.42554	-1.72288
C	-5.36215	1.63863	-0.13924
C	-3.02081	2.27038	-0.83774
S	-4.09257	2.66359	0.50274
C	-5.99203	0.31455	-2.20443
H	-5.89475	-0.76978	-2.04990
H	-5.81754	0.51825	-3.26642
H	-7.01761	0.60131	-1.95655
O	-3.05878	0.98624	-2.86006
C	-2.97401	-0.44244	-3.04775
C	-1.81786	-1.03103	-2.22398
H	-2.79096	-0.57561	-4.11637
H	-3.89779	-0.96046	-2.77948
N	-1.78490	-2.48410	-2.34545
H	-1.94205	-0.79101	-1.16623
H	-0.85697	-0.63034	-2.54967
C	-2.30947	-3.34581	-1.45483
N	-2.22623	-4.57794	-1.97142
C	-1.74152	-4.49062	-3.26580
C	-1.45949	-3.18293	-3.50426
H	-1.04766	-2.68857	-4.36916
H	-1.63594	-5.36299	-3.89021
H	-2.58253	-3.14794	-0.42614
C	-2.87657	-5.73809	-1.36286
H	-2.73436	-5.68099	-0.28101

H	-2.42490	-6.64510	-1.76971
H	-3.94360	-5.67906	-1.59666
C	-0.89921	3.31679	0.13368
C	0.48925	3.36833	-0.19048
C	-1.63494	2.67517	-0.85739
C	0.83225	2.80037	-1.39731
S	-0.59879	2.20881	-2.20617
C	-1.40739	3.86200	1.43808
H	-2.21225	4.59077	1.29516
H	-0.58744	4.36115	1.95990
H	-1.79480	3.07014	2.09045
O	1.39880	3.92602	0.67981
C	2.34341	3.00946	1.23939
C	3.63257	3.80450	1.45276
H	2.53627	2.17190	0.56855
H	1.95089	2.59900	2.17773
N	4.78973	2.91439	1.58670
H	3.57248	4.46081	2.32585
H	3.80282	4.41740	0.56768
C	4.86281	1.84372	2.38880
N	6.03308	1.23599	2.17406
C	6.73553	1.92558	1.19870
C	5.95121	2.97684	0.82742
H	6.09315	3.74275	0.08363
H	7.68411	1.54308	0.83614
H	4.08066	1.47436	3.03017
C	6.44764	-0.01744	2.81104
H	5.56935	-0.66384	2.86302
H	6.84076	0.18937	3.81000
H	7.22555	-0.46034	2.18271
C	2.80236	1.32528	-2.03411
C	4.19084	1.47774	-2.37318
C	2.17641	2.54570	-1.89739
C	4.59429	2.77643	-2.52063
S	3.27868	3.87445	-2.24494
H	5.57746	3.12627	-2.80206
C	2.17225	-0.01684	-1.80689
H	2.49854	-0.44721	-0.85196
H	2.44374	-0.70531	-2.61557
H	1.08529	0.06071	-1.76971
O	5.02530	0.40238	-2.54632
C	5.46191	-0.23341	-1.33243
C	5.35899	-1.73677	-1.58400
H	4.82829	0.04584	-0.48442
H	6.50038	0.04156	-1.11817
N	5.95140	-2.50418	-0.48681
H	5.88828	-1.99470	-2.50421
H	4.31691	-2.04275	-1.68695
C	7.23365	-2.88522	-0.42756
N	7.44089	-3.49701	0.74294
C	6.26528	-3.44331	1.48007
C	5.32790	-2.82228	0.71265
H	4.31228	-2.51057	0.92724
H	6.20343	-3.85499	2.47438
H	7.97428	-2.71969	-1.19005
C	8.76489	-3.85892	1.24537
H	9.26073	-4.52453	0.53581
H	8.64502	-4.37425	2.19880
H	9.33801	-2.93293	1.36160
Cl	-2.41687	-4.15221	1.76210
Cl	-5.03126	-3.03828	-1.90860
Cl	2.98640	-0.54429	1.70329
Cl	8.82736	-0.53680	0.26309

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C₆ ($\bar{\theta} = 49^\circ$) CPT conformer Energy: -3690966.9531361 Ha

C	8.01707	-2.55875	0.71263
C	6.79408	-1.85488	0.41652
C	7.90691	-3.88146	0.38167
C	5.78922	-2.64963	-0.10132
S	6.35423	-4.30391	-0.26388
H	8.66492	-4.64425	0.49946
C	9.21787	-1.95012	1.38001
H	9.86707	-1.39090	0.69266
H	9.82773	-2.73031	1.84534
H	8.90431	-1.25506	2.16826
O	6.56807	-0.54467	0.74690
C	7.41150	0.42643	0.11754
C	7.23131	1.71099	0.92143
H	7.09364	0.58794	-0.91798
H	8.45863	0.11069	0.10824
N	8.02503	2.78380	0.30997
H	7.56734	1.56431	1.95126
H	6.18622	2.02944	0.91880
C	9.35862	2.73699	0.18165
N	9.73997	3.80167	-0.53192
C	8.61905	4.55287	-0.86000
C	7.53600	3.91082	-0.33662
H	6.47122	4.11234	-0.36164
H	8.69271	5.46232	-1.43442
H	10.03990	1.90732	0.43800
C	11.12704	4.03584	-0.93768
H	11.58191	4.80145	-0.30325
H	11.13861	4.36467	-1.97890
H	11.65980	3.08302	-0.84127
C	3.87889	-1.28330	-1.13755
C	2.45113	-1.34115	-1.17056
C	4.40610	-2.31628	-0.38922
C	1.88283	-2.38211	-0.46126
S	3.14036	-3.34795	0.27147
C	4.66259	-0.24227	-1.87680
H	4.76521	0.67971	-1.29088
H	4.15459	0.01734	-2.81128
H	5.66304	-0.61393	-2.11367
O	1.68414	-0.45727	-1.90036
C	1.45778	0.80800	-1.28201
C	0.47273	0.66318	-0.11027
H	1.02764	1.44784	-2.05674
H	2.40357	1.25319	-0.95166
N	0.23098	1.95997	0.53640
H	0.86473	-0.03615	0.63126
H	-0.48986	0.28646	-0.45765
C	1.19603	2.83744	0.84538
N	0.61918	3.90341	1.41007
C	-0.75114	3.69602	1.47376
C	-0.99942	2.47354	0.92335
H	-1.94240	1.94940	0.79727
H	-1.42601	4.42314	1.89556
H	2.27288	2.77320	0.63174
C	1.36564	5.08573	1.84446
H	1.32831	5.16795	2.93362
H	0.92466	5.97643	1.39132
H	2.39923	4.96985	1.50681
C	-0.22488	-2.82814	0.90546
C	-1.63711	-2.85811	0.68756

C	0.46658	-2.63556	-0.27659
C	-2.02759	-2.71008	-0.62831
S	-0.62020	-2.53711	-1.64901
C	0.38151	-2.91006	2.27622
H	1.30145	-2.32205	2.34009
H	0.63833	-3.94229	2.54376
H	-0.33010	-2.54969	3.02473
O	-2.49805	-2.99532	1.75283
C	-3.47502	-1.96374	1.91186
C	-4.73245	-2.64829	2.45055
H	-3.70389	-1.47229	0.96644
H	-3.09388	-1.20109	2.60204
N	-5.92227	-1.81468	2.25335
H	-4.63765	-2.90513	3.50956
H	-4.88855	-3.56561	1.88324
C	-6.03432	-0.52029	2.58220
N	-7.23722	-0.09018	2.19082
C	-7.92074	-1.12987	1.58153
C	-7.09174	-2.21151	1.61792
H	-7.20935	-3.21179	1.23636
H	-8.89255	-0.95505	1.13177
H	-5.26093	0.10089	3.00245
C	-7.71300	1.28948	2.32728
H	-6.86981	1.94825	2.11170
H	-8.08553	1.45025	3.34257
H	-8.51971	1.42896	1.60219
C	-4.00475	-1.52489	-1.71567
C	-5.39821	-1.77832	-1.96158
C	-3.38443	-2.61634	-1.14933
C	-5.81085	-3.03722	-1.62197
S	-4.49754	-3.97202	-0.98052
H	-6.79992	-3.45507	-1.74550
C	-3.36444	-0.19901	-2.00403
H	-3.61683	0.53256	-1.22488
H	-3.71661	0.18626	-2.96716
H	-2.27715	-0.28766	-2.05137
O	-6.22598	-0.82830	-2.50324
C	-6.72413	0.14244	-1.56620
C	-6.65991	1.48597	-2.29003
H	-6.10464	0.17735	-0.66453
H	-7.75874	-0.09287	-1.29254
N	-7.36314	2.53363	-1.54586
H	-7.12642	1.39599	-3.27395
H	-5.62548	1.80514	-2.42387
C	-8.67362	2.79065	-1.64567
N	-8.98345	3.75934	-0.77780
C	-7.84256	4.08236	-0.05559
C	-6.82345	3.31717	-0.53488
H	-5.79642	3.19165	-0.21207
H	-7.86190	4.82517	0.72533
H	-9.36324	2.29491	-2.30616
C	-10.35437	4.15455	-0.45860
H	-10.86548	4.48378	-1.36568
H	-10.32005	4.97859	0.25470
H	-10.85873	3.27987	-0.03384
Cl	11.41484	0.49687	-0.26781
Cl	4.19249	3.37276	0.02407
Cl	-4.32273	1.63583	1.05673
Cl	-10.12980	0.72339	-0.17431

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C₇ ($\bar{\theta} = 59^\circ$) CPT conformer Energy: -3690951.4706891 Ha

C	-0.08176	-6.94349	-0.82814
C	-0.18432	-5.59478	-0.35558
C	-1.32089	-7.46065	-1.09806
C	-1.47769	-5.11153	-0.27565
S	-2.60996	-6.33972	-0.79181
H	-1.55122	-8.45997	-1.44331
C	1.22693	-7.66765	-0.95831
H	1.81262	-7.29567	-1.80899
H	1.07250	-8.74026	-1.10597
H	1.83817	-7.52521	-0.06041
O	0.89965	-4.88753	0.11313
C	1.69872	-4.17424	-0.83218
C	2.34852	-3.04476	-0.03065
H	1.07685	-3.76281	-1.63380
H	2.45358	-4.83846	-1.27334
N	2.91822	-1.99261	-0.87558
H	3.15557	-3.42575	0.60323
H	1.57705	-2.57983	0.58358
C	3.84468	-2.18837	-1.82250
N	4.33171	-1.00040	-2.19734
C	3.75163	-0.00822	-1.41726
C	2.86764	-0.63074	-0.58967
H	2.19320	-0.24039	0.15355
H	4.07639	1.01985	-1.49778
H	4.15055	-3.13991	-2.21652
C	5.43101	-0.81444	-3.14384
H	5.92916	0.12701	-2.89035
H	5.04896	-0.78660	-4.16819
H	6.12526	-1.64773	-3.01550
C	-2.71324	-3.34911	1.13826
C	-2.70264	-1.91349	1.25101
C	-1.87594	-3.77340	0.12860
C	-1.90204	-1.26526	0.33986
S	-1.14138	-2.42595	-0.71818
C	-3.49064	-4.24254	2.05625
H	-4.51451	-4.39455	1.68457
H	-3.55320	-3.79412	3.05349
H	-3.01059	-5.22175	2.13993
O	-3.35895	-1.22326	2.24143
C	-4.76505	-1.06583	2.01681
C	-5.01340	-0.06947	0.87375
H	-5.17498	-0.68567	2.95558
H	-5.22682	-2.03612	1.79604
N	-6.43857	-0.04812	0.51724
H	-4.44585	-0.37455	-0.00694
H	-4.71684	0.94825	1.13267
C	-7.14281	-1.15249	0.23364
N	-8.40291	-0.78268	-0.01590
C	-8.50349	0.59744	0.09957
C	-7.26597	1.06301	0.43542
H	-6.86980	2.06178	0.57282
H	-9.43269	1.11777	-0.06903
H	-6.81522	-2.21444	0.25675
C	-9.46477	-1.74152	-0.32723
H	-9.79969	-1.60261	-1.35847
H	-10.30235	-1.58833	0.35737
H	-9.04989	-2.74588	-0.19243
C	-1.59148	1.09133	-0.62694
C	-0.61659	2.12774	-0.48951
C	-1.39781	0.10017	0.30340
C	0.32133	1.94878	0.50571
S	-0.04866	0.46886	1.37102
C	-2.65227	1.10519	-1.68639

H	-3.04616	0.09897	-1.85386
H	-2.24682	1.48080	-2.63170
H	-3.48297	1.75982	-1.38991
O	-0.59157	3.20822	-1.35045
C	-1.28144	4.33258	-0.81109
C	-1.53816	5.27857	-1.98246
H	-0.67332	4.82429	-0.04041
H	-2.23156	4.01295	-0.36430
N	-2.43269	6.36318	-1.55384
H	-2.01299	4.73140	-2.79990
H	-0.61278	5.72426	-2.35181
C	-3.67453	6.14335	-1.10033
N	-4.17321	7.30848	-0.67607
C	-3.22992	8.30588	-0.86996
C	-2.13244	7.70914	-1.41728
H	-1.17893	8.11426	-1.71664
H	-3.41885	9.33354	-0.60359
H	-4.17490	5.16858	-0.95887
C	-5.49834	7.43638	-0.06138
H	-5.84517	6.42893	0.18427
H	-6.18778	7.92047	-0.75718
H	-5.41115	8.02998	0.85055
C	2.42388	2.64224	1.78506
C	3.66439	3.29836	1.48726
C	1.55863	2.67243	0.70690
C	3.74095	3.81412	0.22308
S	2.28453	3.52025	-0.66262
H	4.58549	4.28730	-0.25601
C	2.17383	1.98772	3.11415
H	2.81271	2.44387	3.87465
H	2.40894	0.91481	3.09198
H	1.13013	2.08419	3.42665
O	4.65588	3.37197	2.43846
C	5.90205	2.78538	2.05552
C	5.82436	1.26323	2.23371
H	6.65170	3.22077	2.72219
H	6.16052	3.00065	1.01340
N	7.03589	0.62819	1.72150
H	4.98831	0.87413	1.64915
H	5.67876	0.99135	3.28328
C	7.07129	-0.16147	0.63930
N	8.34915	-0.40494	0.33946
C	9.15846	0.29582	1.21700
C	8.33870	0.94278	2.08802
H	8.55894	1.57880	2.92942
H	10.23344	0.26201	1.14627
H	6.23110	-0.64209	0.16347
C	8.77517	-1.14825	-0.84398
H	8.10895	-2.00952	-0.95392
H	9.80394	-1.48034	-0.69549
H	8.70750	-0.48369	-1.70979
Cl	5.96195	-3.13245	-0.19093
Cl	-6.83965	-4.21907	0.56972
Cl	-5.03369	3.64614	0.16544
Cl	6.49279	1.98819	-1.33925

9. Dihedral angle dependence

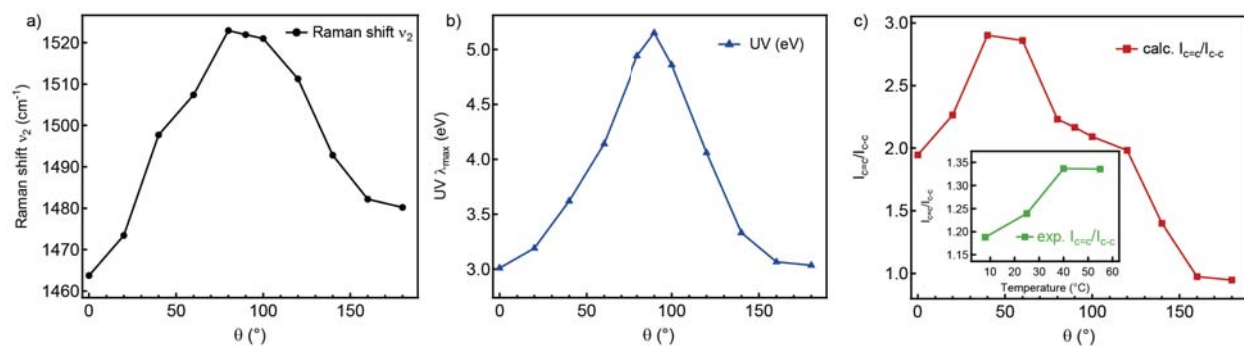


Figure S9: Dihedral angle dependence (a) of the computed ν_2 band maximum, (b) of the vertical excitation energies (computed at the CAM-B3LYP/6-311G*level) and (c) of the computed $\frac{I_{\nu_{\text{C}=\text{C}}}}{I_{\nu_{\text{C}-\text{C}}}}$ Raman intensity ratio. The inset shows the experimental $\frac{I_{\nu_{\text{C}=\text{C}}}}{I_{\nu_{\text{C}-\text{C}}}}$ ratio as a function of temperature.

10. TA spectra at the different excitation wavelengths

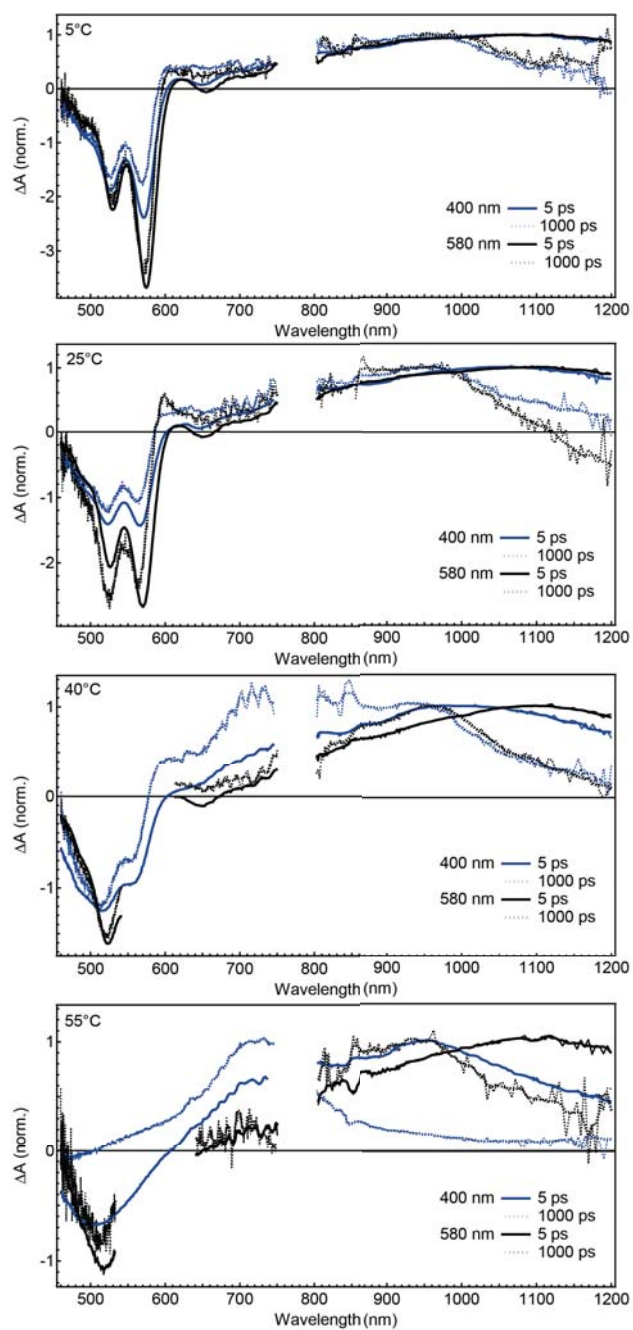


Figure S10. Normalized TA spectra for CPT at different temperatures, compared at 5 ps and 1000 ps after photoexcitation at 400 nm or 580 nm.

11. Dynamic Light Scattering (DLS) measurements

DLS measurements were performed on a DelsaMax Pro Beckman Coulter instrument at room temperature. Each result indicated in the following table is the average value over 5 measurements.

Table S1 DLS results for different concentrations of CPT in PBS

Monomeric concentration (M)	Diameter (nm)
$1.5 \cdot 10^{-5}$ (sonicated for 1h)	137.0
$1.5 \cdot 10^{-5}$	152.2
$7.5 \cdot 10^{-5}$	121.8
$1.5 \cdot 10^{-4}$	122.3

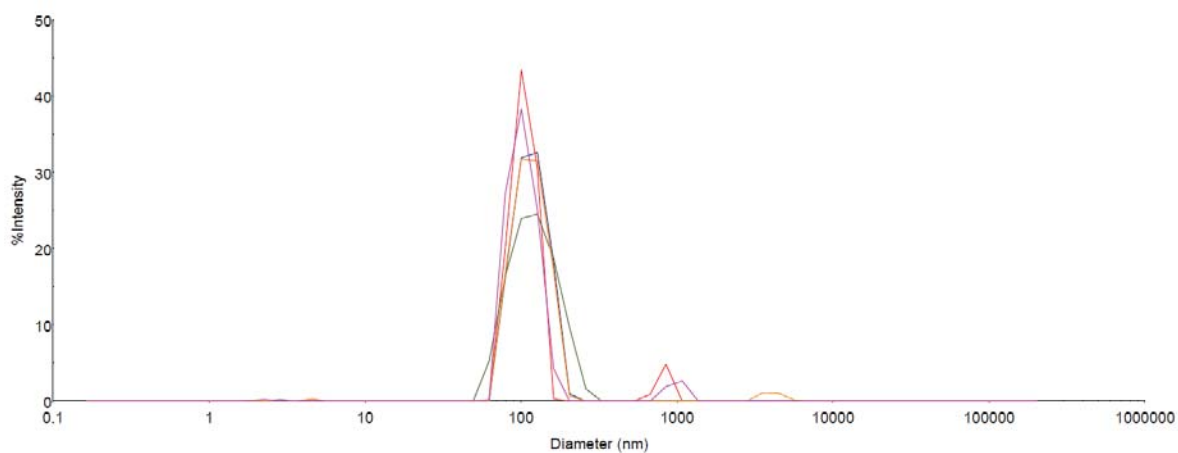


Figure S11 Size distribution of CPT in PBS ($1.5 \cdot 10^{-4}$ M, monomeric basis) obtained by the DLS measurement.

12. Fluence dependence of polaron formation

Figure S11 shows the TA dynamics probed in the GSB obtained for CPT at 5°C with 400 nm excitation with two different laser fluences. The dynamics and long-lived offset (related to polaron yield) are independent of the excitation intensity, and the signal amplitude scales linearly with fluence. This shows that exciton-exciton annihilation does not play a role in polaron formation within the investigated fluence range.

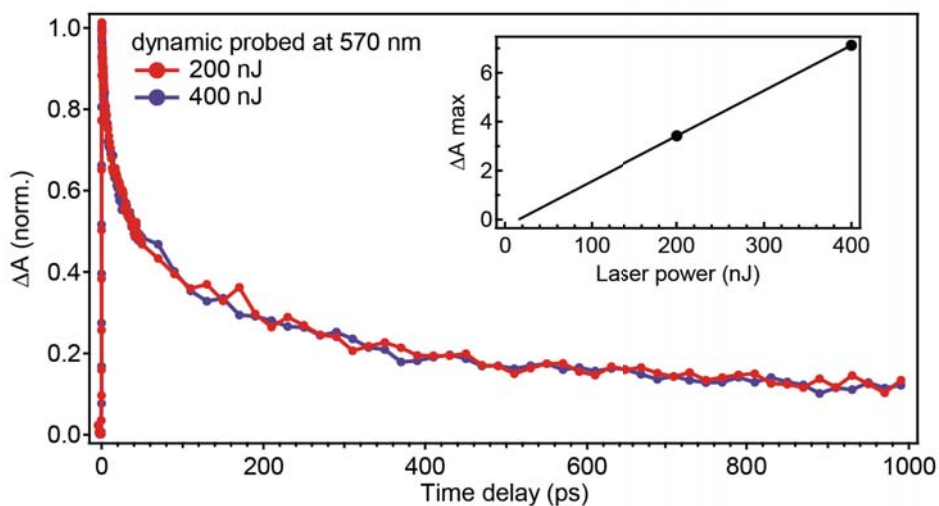


Figure S12 Transient absorption dynamics for CPT (1.5 · 10⁻⁴ M on a monomeric unit basis in PBS) at 5°C with 400 nm excitation, probed at 570 nm (GSB) and recorded with two excitation fluences. The maximum signal amplitude as a function of pulse energy is shown in the inset.